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(54) Title: **WATER-SOLUBLE LIGAND-BINDING PROTEINS AND ANALOGS OF LIGAND-GATED ION CHANNELS, CRYSTALS THEREOF AND THEIR USE FOR SCREENING LIGANDS OF LIGAND-GATED ION CHANNELS**

(57) Abstract: Provided are water-soluble ligand-binding proteins derived from molluscs and analogs of ligand-gated ion channels, crystals thereof and their use for screening ligands of ligand-gated ion channels. In particular, water-soluble ligand-binding proteins are provided that are capable of forming multimers and are amenable to crystallization. The crystal structure of one of these proteins, an acetylcholine binding protein (AChBP) is provided, which can be used to generate 3D models of the extracellular ligand-binding domain of ligand-gated ion channels and thus for screening of drugs that act on these ion channels. Furthermore, chimeric proteins are provided that are capable of binding a ligand of a ligand-gated receptor, and comprising at least the amino acids of the AChBP determining solubility of the AChBP, in the same positions as in the AChBP, and furthermore comprising amino acids determining binding to said ligand.

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5 **WATER-SOLUBLE LIGAND-BINDING PROTEINS AND ANALOGS OF LIGAND-
GATED ION CHANNELS, CRYSTALS THEREOF AND THEIR USE FOR
SCREENING LIGANDS OF LIGAND-GATED ION CHANNELS**

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SUMMARY OF THE INVENTION

Novel water-soluble ligand-binding proteins have been identified and isolated, which have a ligand-binding profile substantially similar to that of ligand-gated ion channels. DNA molecules encoding such proteins have been cloned and characterized. The biological and structural properties of these proteins are disclosed, as is the amino acid and nucleotide sequence. The recombinant DNA molecules, and portions thereof, are useful for isolating homologues of the DNA molecules, identifying and isolating genomic equivalents of the DNA molecules, and identifying, detecting or isolating mutant forms of the DNA molecules. Using a recombinant expression system functional DNA molecules encoding the water-soluble ligand-binding proteins as well as chimeras have been functionally produced. Furthermore, the water-soluble ligand-binding proteins could be crystallized revealing the three dimensional (3D) structure and enabling the modeling of the 3D structure of the ligand-binding domain of ligand-gated ion channels. The invention is further in the field of the development of new drugs that are capable of selectively intervening in neuronal signaling pathways. The invention is more in particular concerned with providing new analogues of the channel-coupled receptors, crystal structures thereof and to their use in screening ligands for these receptors.

30 Several documents are cited throughout the text of this specification either by name or are referred to by numerals within parenthesis. Full bibliographic citations may be found at the end of the specification immediately preceding the claims. Each of the documents cited herein (including any manufacturer's specifications, instructions, etc.) are hereby incorporated herein by reference; however, there is no admission
35 that any document cited is indeed prior art as to the present invention.

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BACKGROUND OF THE INVENTION

The communication in the central nervous system (CNS) occurs through a complex interaction of electrical and chemical signals. Molecules bearing chemical information are called neurotransmitters. The chemical information is converted in electric currents on the post-synaptic membrane, which is specialised in recognising and binding neurotransmitters by means of protein receptors. The specific binding of a ligand to one type of such receptors, the ionotropic receptors, induces a fast opening of the ion channel coupled to the receptor. An important group of ionotropic receptors is the superfamily of the channel-coupled receptors, also referred to as ligand-gated receptors, including the 7-amino-butyric acid (GABA_A) receptor, the glycine receptor, the serotonin-3 (5-HT₃) receptor and both neuronal and muscle-type nicotinic acetylcholine receptors (nAChR). These receptors share certain structural features such as (1) a 15-residue cysteine loop between amino acids 128 and 142 corresponding to the Torpedo AChR α unit, (2) four trans-membrane domains, (3) similar subunit arrangements, and (4) homologies in amino acid sequence. Activation of these receptors causes a change in electrical current and hyperpolarisation of the cell membrane and consequently an inhibition of the electrical activity of the cell. The GABA_A receptor and the glycine receptor are coupled to a chloride-selective channel, and thus the inhibition of the electrical activity leads to inhibition of the cell response. On the other hand, activation of the 5-HT₃ receptor and the nAChRs provokes an excitatory response on the cell because they are connected to a cation-selective channel (Na⁺, K⁺, Ca²⁺). The AChRs are the best studied of the ligand-gated receptors; for a review, see Arias, Brain Research Reviews, 25 (1997)133-191 and Arias, Neurochem. Int. 36 (2000), 595-645). Mutations in these ligand-gated ion-channels (LGICs) lead to diseases such as congenital myasthenia gravis, epilepsy, startle syndrome and alcohol sensitivity (Vafa and Schofield, Int. Rev. Neurobiol. 42, 285-332; 1998). NACHRs mediate nicotine addiction in chronic tobacco users. Since nicotine binding to these receptors also has a positive effect on Alzheimer's disease, Parkinson's disease and schizophrenia these receptors present an important drug target (Paterson and Nordberg, A. Neuronal nicotinic receptors in the human brain. Prog. Neurobiol. 61, 75-111; 2000).

The development of new active compounds that can selectively or - as the case may be - a-selectively bind to the channel-coupled receptors, is of utmost importance for the understanding of the processes occurring in the nervous system and for the treatment of disturbances of neural conditions. The development of such active compounds requires the availability of a reliable model system for the corresponding receptors. The primary structural features (amino acid sequences) of the various

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receptors have been largely elucidated by now. Certain subunits of the AChRs have been found to be determinant in the pharmacological specificity or affinity of the receptor for its ligand (Corringer et al., J. Neuroscience 18 (1998), 648-657). However, the study of the ligand binding properties of the receptor proteins is
5 hampered by the fact that the spatial structure of the proteins - which is decisive in the binding of ligands - is still unknown. This is partly because crystallisation of the receptor proteins has been unsuccessful up to now.

The above-defined technical problem is solved by the present invention by providing the embodiments characterized in the claims.

10 Accordingly, in one aspect the present invention relates to a water-soluble protein derived from a mollusc being capable of binding a ligand of a ligand-gated receptor.

It has been found according to the invention that acetylcholine-binding proteins (AChBP) of certain molluscs show a surprising structural similarity with the channel-coupled receptors on the one hand and have interesting physical properties, such as
15 water-solubility, on the other hand. The molluscan AChBPs are capable of forming multimers, especially pentamers, and of binding specific toxins such as α -bungarotoxin. These multimers may be homogeneous (identical units) or heterogeneous (different units). These properties make them eminently suitable as
20 model systems for studying the binding of candidate ligands to the channel-coupled receptors. It has been possible to produce these molluscan AChBPs in recombinant systems, thus allowing convenient and large-scale production thereof. Moreover, it is feasible to construct hybrid proteins sharing the physical properties of the mollusc AChBP with the pharmacological properties of the (human) channel-coupled
25 receptors, thus providing new dedicated tools for screening ligands for these receptors.

The AChBP is a naturally occurring analogue of the extracellular domains of the α -subunits of the neuronal nicotinic acetylcholine receptors (nAChRs). In contrast to the
30 nAChRs, it lacks domains to form a transmembrane ion channel, but alike the nAChRs it assembles into a homo-pentamer (Figure 6). Moreover, AChBP has ligand-binding characteristics that are typical for a nicotinic receptor. The 3-dimensional structure of AChBP was solved by X-ray crystallography at 2.7Å resolution (current $R_{\text{factor}} = 27.9\%$, $R_{\text{free}} = 30.0\%$). In crystals, as in solution, AChBP
35 forms a stable homo-pentamer with dimensions comparable to those of the ligand-binding domain of the nAChR, as determined in EM studies by Unwin, Struct. Struct. Biol 121 (1998), 181-190. The high-resolution crystal structure of AChBP, along with

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biochemical and pharmacological data, supports the extrapolation of AChBP as a good mimic of ligand-binding domains of ligand-gated ion channels including nAChR, 5-HT3R, GABA_AcR and GlyR.

Four AChBPs according to the present invention are exemplified herein, isolated and
5 cloned from the CNS of *Lymnaea stagnalis* (L-AChBP_T1 and L-AChBP_T2) and *Bulinus truncatus* (B-AChBP_T1 and B-AChBP_T2). L-AChBP_T1 and 2 are 229 amino acid proteins with a signal sequence of 19 amino acids (224 and 21 amino acids, respectively, for B-AChBP_T1 and 2; see also Figure 1) and have sequence homology with the extracellular domains of the subunits of ligand-gated ion channels
10 (Figure 3), in particular with those of the nAChRs (Figure 4 and 5). The mass of the purified AChBP from *Lymnaea* has been determined by mass-spectrometry. The glycosylated form has a mass of about 24720 Da and the de-glycosylated form of about 23832 Da. In SDS-PAGE the glycosylated AChBP migrates between the 14 and 26 kDa marker proteins. Hydrophobicity plots of the AChBPs are shown in
15 Figure 2, which reveal those regions of the ligand-binding proteins that are particularly hydrophilic and thus may be replaced at least in part or essential amino acids thereof in the ligand-binding domain of the ligand-gated ion channel. Sequence conservation is particularly high in the so-called loop areas (reviewed by Arias, Neurochem. Int. 36 (2000), 595-645), which contain the residues involved in ligand-
20 binding. The cysteine residues characteristic for the Cys-loop family of ligand gated receptors are conserved in AChBP. Also the double cysteine typically found in the alpha subunits of the nAChR is present. AChBP protein sequence ends at the position where in the nAChRs the first predicted transmembrane domain would start. The ligand-binding characteristics of AChPBs are described in Example 4 and
25 summerized in Table 2.

The terms "channel coupled receptors", "ligand-gated receptor", "ligand-gated ion channel" are used interchangeable herein. However, in context with the natural occurring, in particular human molecules the term "ligand-gated ion channel" is
30 preferably used. The water-soluble ligand-binding protein of the invention can also be characterized as a ligand-binding protein having at least 10%, more preferably at least 12%, still more preferably at least 15% and most preferably at least 20% amino acid sequence identity to a vertebrate ligand-gated ion channel but missing any trans-membrane domain. A ligand-gated receptor of the present invention is
35 characterized by having substantially the same ligand-binding characteristics of a vertebrate, preferably mammalian, most preferably human ligand-gated ion channel but comprising at least one alteration in the original amino acid sequence, said

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alteration resulting in the presence of an amino acid determining or contributing to the water-solubility of the water-soluble ligand-protein found in molluscs, in particular snails such as those described in more detail below.

- 5 The terms "ligand-binding protein", "ligand-binding domain" and "ligand-binding receptor" are meant to at least include the portion of a water-soluble ligand-binding protein or corresponding modified ligand-gated ion channel required for binding a ligand. Minimally the ligand-binding domain consists of a peptide containing that domain. However the use of this term is meant to include a ligand-binding domain or
10 protein that is comprised by a larger portion of, for example, ligand-gated ion channel, such as a fully reconstituted nicotinic acetylcholine receptor.

As shown in Figure 3 the nicotinic acetylcholine receptor (nAChR) belongs to a well-understood member of the ligand-gated ion channels superfamily. The members of
15 this signaling protein group, including 5-HT₃, glycine, GABA_A, and GABA_C receptors, are thought to share common secondary, tertiary, and quaternary structures on the basis of a high degree of sequence similarity. Therefore, it is expected that the novel findings in respect to the exemplified AChBP equally apply to the other members of the mentioned ligand-gated ion channels superfamily. Thus, either water-soluble
20 protein being capable of binding a ligand of any of those ligand-gated ion channels may be found in molluscs or the present 5-HT₃, GABA_A, and glycine receptors can be modified such as to substantially retain their binding affinity.

Accordingly, the ligand of the water-soluble ligand-binding protein is preferably acetylcholine, gamma-amino-butyric acid (GABA), glycine, nicotine or serotonin.
25 Isolation of such water-soluble ligand-binding proteins can be done as described in Example 1 for the AChBP of the present invention. Instead of α -bungarotoxin other known ligands or can be used for affinity purification. Most preferably, water-soluble ligand-binding protein of the invention is a acetylcholine-binding protein (AChBP). Preferably, the ligand-binding protein displays substantially the binding
30 characteristics shown in Table 2.

The acetylcholine-binding proteins to be used according to the invention are originally derived from aquatic molluscan species, especially species from the class of the snails (Gastropoda), in particular from the order of the lunged snails (Pulmonata). The order of the Pulmonata is divided into the suborders of the Basommatophora
35 (mostly aquatic snails), Systellommatophora and Stylommatophora (mostly land snails). The Basommatophora include the families of the Acroloxidae (e.g. genus *Acroloxus*), Lymnaeidae (e.g. genera *Galba*, *Stagnicola*, *Radix* and *Lymnaea*),

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Physidae (e.g. genera Physa and Aplexa) and Planorbidae (e.g. genera Planorbis, Anisus, Ancyclus, Gyraulus, Biomphalaria and Bulinus). Examples of suitable species are *Lymnaea stagnalis* (pond snail) and *Bulinus truncatus*. The isolation of the AChBPs from these snails, cloning of the cDNA encoding these AChBPs and their
5 characterization including the full amino acid sequences is described in the examples. The cDNA and amino acid sequences of the AChBPs of *Lymnaea stagnalis* are depicted in SEQ ID Nos. 1 and 2 (L-AChBP_T1) and SEQ ID Nos. 3 and 4 (L-AChBP_T2). Those of *Bulinus truncatus* are depicted in SEQ ID Nos. 5 and 6 (B-AChBP_T1) and SEQ ID Nos. 7 and 8 (B-AChBP_T2). Features of these
10 proteins are further described in the examples and the accompanying figures.

While a water-soluble ligand-binding protein derived from a Pulmonata species, preferably from a Basommatophora species is preferred, it will be appreciated that the present invention generally relates to any water-soluble protein being capable of
15 binding a ligand of a ligand-gated receptor comprising an amino acid sequence selected from the group consisting of:

- (a) an amino acid sequence as depicted in any one of SEQ ID Nos. 2, 4, 6 or 8 or a functional equivalent thereof, or a fragment of at least 5 continuous amino acids thereof;
- 20 (b) an amino acid sequence having at least 30% amino acid identity to the amino acid sequence of any one of SEQ ID Nos. 2, 4, 6 or 8; and
- (c) an amino acid sequence resulting in a protein which is detectable by a monoclonal or polyclonal antibody which recognises, preferably with a binding affinity of at least $10^{-7}M$, a protein comprising an amino acid sequence of (a)
25 or (b).

Identity or similarity, as known in the art, are relationships between two or more polypeptide sequences or two or more polynucleotide sequences, as determined by comparing the sequences. In the art, identity also means the degree of sequence
30 relatedness between polypeptide or polynucleotide sequences, as the case may be, as determined by the match between strings of such sequences. Both identity and similarity can be readily calculated (Computational Molecular Biology, Lesk, ed., Oxford University Press, New York, 1988; Biocomputing: Informatics and Genome Projects, Smith, ed., Academic Press, New York, 1993; Computer Analysis of
35 Sequence Data, Part I, Griffin and Griffin, eds., Humana Press, New Jersey, 1994; Sequence Analysis in Molecular Biology, von Heinje, Academic Press, 1987; and Sequence Analysis Primer, Gribskov and Devereux, eds., M Stockton Press, New

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York, 1991). While there exist a number of methods to measure identity and similarity between two polynucleotide or two polypeptide sequences, both terms are well known to skilled artisans (von Heinje, supra; Gribskov and Devereux, supra; and Carillo and Lipman SIAM J. Applied Math. 48 (1988), 1073). Methods commonly employed to determine identity or similarity between sequences include, but are not limited to those disclosed in Carillo and Lipman; see supra. Preferred methods to determine identity are designed to give the largest match between the sequences tested. Methods to determine identity and similarity are codified in computer programs. Preferred computer program methods to determine identity and similarity between two sequences include, but are not limited to, GCG program package (Devereux et al., Nucleic Acids Research 12 (1984), 387), BLASTP, BLASTN, psi BLAST and FASTA (Atschul et al., J. Molec. Biol. 215 (1990), 403).

In another embodiment, the present invention relates to a water-soluble protein being capable of binding a ligand of a ligand-gated receptor comprising

- (a) at least the amino acids of the water-soluble protein described above determining solubility of said protein, in the same or corresponding positions as in said protein; and
- (b) at least 4 amino acids determining binding to said ligand.

Protein expression studies have shown that wild-type AChBP of the mollusc *Lymnaea stagnalis* can be produced in *Pichia pastoris* yeast. The yeast cells express AChBP in a homopentameric form and secrete the protein complex into the medium. The large amounts of AChBP per volume of medium produced (up to 2 mg per liter medium) and the large volumes of yeast that can be cultured allow a large-scale production of AChBP. Besides the wild-type AChBP, various AChBP mutants have been produced in *Pichia pastoris*. These include mutants containing the following single point mutations (the numbers refer to the amino acid position in the AChBP sequence of *Lymnaea stagnalis* depicted in SEQ ID No. 2 counted from the first amino acid of the signal peptide; the letter before the number indicates the original amino acid and the letter after the number indicates the mutant amino acid) N85D, H164Y, D194N, Y204P, Y211P and D213N.

Thus the invention pertains to water-soluble proteins derived from molluscan, preferably acetylcholine binding proteins (AChBP's), which are capable of forming multimers, and are capable of binding a ligand of a ligand-gated receptor. These proteins comprise, on the one hand, at least of the amino acids of the AChBP determining solubility of the AChBP in the same positions as in the AChBP, and, on

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- the other hand, amino acids determining binding to the ligand of the ligand-gated receptor. The degree of identity with the molluscan AChBP sequence can be defined by amino acid identity, of at least 15%, preferably 20%, more preferably 30%, still more preferably 40%, preferably at least 50 or even at least 60%, preferably more than 70%, more preferably more than 80% and most preferably at least 90% identity, or more, as determined, e.g., using the art-known BLAST algorithm. The amino acids determining binding to the ligand should comprise at least 4 amino acids, preferably at least 6 or even at least 8 amino acids, including a series of at least 3 or 4 amino acids, corresponding to the receptor sequence and preferably differing from the corresponding AChBP amino acids. Preferred embodiments of these proteins are further defined below. Usually, the water-soluble ligand-binding protein or domain as part of a for example chimeric ligand-gated ion channel will comprise 200-240 amino acids. The ligand is preferably acetylcholine, nicotine, lophotoxin, d-tubocurarine, carbamylcholine, galanthamine or epibatidine.
- Said ligand-gated receptor can be derived from an arthropod (preferably insect), a plant (preferably a higher plant, most preferably a seed plant) or a chordate (preferably a mammalian, most preferably human), preferably said ligand-gated receptor is a nicotinic acetylcholine receptor.
- Usually, the said amino acids in the water-soluble ligand-binding proteins of the invention, which determine solubility are in the same positions as in the AChBP having the amino acid sequence as depicted in any one of SEQ ID Nos. 2, 4, 6 or 8. The solubility determining regions are based on solvent accessibility in structure. The respective amino acid residues can be chosen for example according to Figure 10 or 11 in which the solvent accessible regions are indicated. Preferably, the water-soluble ligand-binding protein of the invention comprises an amino acid sequence having at least 40% amino acid identity to the amino acid sequence of the mature AChBP comprising the amino acid sequence of any one of SEQ ID Nos. 2, 4, 6 or 8, in which the ligand binding amino acids have been replaced with the corresponding amino acids of a ligand-gated receptor.
- In one embodiment of the protein of the invention said solubility-determining amino acids (a) comprise hydrophilic amino acids (Asp, Glu, Arg, Lys) from the sequences 20-44, 73-81, 86-92, 112-120, 135-152, 166-189, 196-20, 209-213, and/or 219-227 of SEQ ID No. 2.
- The amino acid sequences of L-AChBP_T1 (SEQ ID No. 2) and T2 (SEQ ID No. 4) are almost similar. For the sake of clarity, reference is always made to L-AChBP_T1 (SEQ ID No. 2). However, all references to amino acid residues within are valid for

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both T1 and T2, with the noticeable exceptions of Arg(167) becoming Gly(167) and and Thr(203) becoming Ile(203). Furthermore, regarding the amino acid residues (domains) from L-AChBP_T1 and the corresponding residues from B-AChBP the following list provide those amino acid positions in which L-AChBP and B-AChBP differ. All amino acid residue numbers below correspond to their position within the amino acid sequence of the immature protein (numbering starting at methionine (1). One could also start numbering at the start of the amino acid sequence of the mature sequence (L(1)DRAD for L-AChBP and Q(1)IRW for B-AChBP). When using this second method (1st amino acid of the mature seq. = position 1) simply subtract 19 from the L-AChBP position numbers and 21 from the B-AChBP position numbers, for example Asp(36) becomes Asp(17) for L-AChBP and Asp(15) for B-AChBP. For the further embodiments the positions are given for L-AChBP T1 (SEQ ID No. 2) followed by an indication of the corresponding amino acid positions in the amino acid sequence of L-AChBP_T2 (SEQ ID No. 4) and B-AChBP_T1 (SEQ ID No. 6) & B-AChBP_T2 (SEQ ID No. 8) in the form of (L-AChBP_T1&T2 : B-AChBP_T1&T2).

In a preferred embodiment said solubility determining amino acids (a) comprise amino acids Asp(36), Asp(68), Glu(115), Arg(137), Asp(143), Asp(148), Glu(150), Arg(167), Arg(189), Glu(215) of SEQ ID No.2, wherein Asp may be exchanged for Glu and vice versa and Lys may be exchanged for Arg and vice versa (L-AChBP_T1&T2 : B-AChBP_T1&T2; Asp(36) : Asp(36); Asp(68): Asp(68); Glu(115): Glu(116); Arg(137): Arg(138); Asp(143): Asp(144); Asp(148): Asp(149); Glu(150): Glu(151); Arg(167): Gly(167), in L-AChBP_T2 : Lys(168); Arg(189): Lys(190); Glu(215): Glu(216).

In a still more preferred embodiment the water-soluble ligand-binding protein comprises the amino acids Cys(142), Thr(149), Ala(153), Thr(154), Cys(155), Arg(156), Ile(157) and/or Lys(158) of SEQ ID No. 2. (L-AChBP_T1&T2 : B-AChBP_T1&T2; Cys(142): Cys(143); Thr(149): Thr(150); Ala(153): Ala(154); Thr(154): Thr(155); Cys(155): Cys(156); Arg(156): Arg(157); Ile(157): Ile(158); Lys(158): Lys(159). In a further embodiment the water-soluble ligand-binding protein comprises either in addition or alternatively the amino acids (b) Pro(39), Trp(77), Trp(101), Pro(103), Asp(194), and/or Ser(161) of SEQ ID No. 2 (L-AChBP_T1&T2 : B-AChBP_T1&T2; Pro(39): Pro(39); Trp(77): Trp(77); Trp(101): Trp(102); Pro(103): Pro(104); Ser(161): Ser(162); Asp(194): Ser(195).

In a still further embodiment the water-soluble ligand-binding protein comprises either

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in addition or alternatively to the above described embodiments amino acid sequences 165-169 and/or 200-203 of SEQ ID No. 2 have been exchanged with the corresponding sequence of the ligand-gated receptor (L-AChBP_T1&T2 : B-AChBP_T1&T2; His(165)-Iso(169):. Asp(166)-Phe(170) (B-AChBP_T1) : Asp(166)-
5 Leu(170) (B-AChBP_T2); Asn(200)-Thr(203); Iso(203) for L-AChBP_T2: Asn(201)-Lys(204).

The amino acids determining binding to the ligand of the nicotinic acetylcholine receptor include three stretches on the nAChR alpha subunits. These stretches contain amino acids that are conserved throughout the various nAChR alpha
10 subunits and that are essential for ligand binding. These stretches (corresponding to the Torpedo alpha subunit) are (numbering of nAChR α 7 as depicted in SEQ ID No. 9): Trp (108) - Tyr (115), Trp (108) and Tyr (115) being essential; Trp (171) - Tyr (173), the amino acids Trp (171) and Tyr (173) being essential; Tyr (210) - Tyr (217), the amino acids Tyr (210), Cys (212), Cys (213) and Tyr (217) being essential. In the
15 chimeric proteins according to the invention, at least the essential amino acids of at least one of these stretches haven been substituted for the corresponding amino acids. Preferably, the entire stretches have been substituted.

In a particularly preferred embodiment of the invention, the water-soluble ligand-binding protein is capable of binding a ligand of an acetylcholine receptor, wherein in
20 said protein at least one of the amino acid sequences Trp(101) - Tyr(T108), Trp(162) - His(164) and Tyr(204) - Tyr(211) of SEQ ID No. 2 has been exchanged with the corresponding sequence of the acetylcholine receptor (L-AChBP_T1&T2 : B-AChBP_T1&T2; Trp(101)-Tyr(108): Trp(102)-Tyr(109); Trp(162)-His(164): Trp(163)-
25 His(165), (B-AChBP_T1) : Trp(163)-Phe(165) (B-AChBP_T2); Tyr(204)-Tyr(211): Tyr(205)-Tyr(212).

On the basis of homology to the AChBPs, it is possible to change amino acid residues in the original amino acid sequence of the ligand-gated ion channel, which
30 are not critical to ligand-binding or essential for the tertiary and quaternary structure of the receptor but could be substituted to amino acid residues which according to the AChBP in particular the crystal structure contributes to their water-solubility. As a result the ligand-gated ion channel or its ligand-binding domain or the respective monomers and pentamers are for example expected to be more easily expressible in
35 recombinant expression system and more importantly amenable to crystallization, allowing the construction of three-dimensional models of their ligand binding domains.

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Thus, in another embodiment the present invention relates to a method for the production of a water-soluble ligand-gated receptor or a corresponding ligand-binding domain or for improving the water solubility and accessibility to crystallization of such a receptor or domain, said method comprising altering the amino acid sequence of the extracellular domain of a ligand-gated receptor by way of substituting, adding, deleting or modifying at least one amino acid at a position corresponding to an amino acid determining or contributing to the water-solubility of the above-described water-soluble ligand-binding protein of the present invention. The method of the invention can be performed using conventional techniques known in the art, for example, by using amino acid deletion(s), insertion(s), substitution(s), addition(s), and/or recombination(s) and/or any other modification(s) known in the art either alone or in combination. Methods for introducing such modifications in the DNA sequence underlying the amino acid sequence of the ligand-binding domain a ligand-gated ion channel are well known to the person skilled in the art; see, e.g., Sambrook, Molecular Cloning A Laboratory Manual, Cold Spring Harbor Laboratory (1989) N.Y. The resulting ligand-gated receptor or ligand-binding domain retains comparable in vitro and preferably also in vivo ligand-binding activity to that of the ligand-gated ion channel, and more importantly, allow complete crystallization of the protein such that they may be characterized by X-ray crystallography. The X-ray crystallographic data can be used for example for identification and construction of possible therapeutic compounds in the treatment of various disease conditions.

As has been discussed herein before, the ligand-gated ion channel superfamily including nACh, 5-HT₃, glycine, GABA_A, and GABA_C receptors as well as invertebrate glutamate ion-channels and MOD-1 serotonin channel contain extracellular ligand binding domains that are homologous to the AChBP. Many of these receptors are promising drug targets. Therefore, the ligand-gated receptor to be modified is preferably one of those of the mentioned superfamily, most preferably it is nAChR.

Information on the nucleotide and amino acid sequences, structural elements, functional assays of the nACh, 5-HT₃, glycine, GABA_A, and GABA_C receptors can be found in the prior art. For example, the nicotinic receptors at the amino acid level are described in Corringer et al., Annu. Rev. Pharmacol. Toxicol. 40 (2000), 431-458. Means for retrieving nucleotide and amino acid sequences, performing sequence alignments in order to identify the most likely critical amino acid residues are described below and in the examples; for further general information see the review on periplasmic binding protein (PBP), an ancient protein module present in multiple drug receptors by Felder et al., PharmSci. 1(2) (1999).

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In a preferred embodiment of the method of the present invention, said at least one amino acid is altered to the corresponding amino acid of the amino acid sequence depicted in any one of SEQ ID Nos. 2, 4, 6 or 8, or to an equivalent amino acid, preferably in which said solubility-determining amino acids comprise solvent accessible regions in the crystal structure according to Figure 10 or 11. Preferred amino acid sequence positions and amino acid substitutions are described above for the AChBP and can be applied generally in the method of the present invention. It is expected that the insertion of the loop Cys123-Cys136 of the mature AChBP SEQ ID No. 2 into the equivalent region (Cys127-Cys141) in the mature nicotinic $\alpha 7$ homopentamer ligand binding domain creates an easily expressed form of this protein. Likewise, this loop or an equivalent loop from other water-soluble ligand proteins of the present invention can be inserted into the equivalent region of other homopentameric ligand binding domains of ligand gated ion channels such as the glycine receptor and the 5-HT₃ receptor to create an easily expressed form of those proteins.

Thus, in one embodiment, the present invention relates to any one of the above described methods, wherein loop Cys123-Cys136 of SEQ ID No. 2 is inserted into the corresponding region of the ligand binding domain of the ligand-gated receptor.

The above described water-soluble ligand-gated receptor or a corresponding ligand-binding domain are usually prepared by site-directed mutagenesis of the underlying encoding polynucleotide. Once the corresponding polynucleotide has been generated it can be used to express the altered ligand-gated receptor or a corresponding ligand-binding domain. Thus, the method of the present invention commonly comprises

- (a) culturing a host cell transfected with and capable of expressing a polynucleotide comprising a nucleotide sequence encoding the altered amino acid sequence; and optionally
- (b) recovering said water-soluble ligand-gated receptor or corresponding ligand-binding domain from the culture.

Methods for the expression and purification of the water-soluble ligand-gated receptor or corresponding ligand-binding domain of the present invention are described further below. Preferably, the expression system described in Examples 4 and 5, or corresponding expression systems are used.

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The present invention also relates to the a water-soluble ligand-gated receptor and ligand-binding domain obtainable by the above described methods of the invention. Preferably, said water-soluble ligand-gated receptor exhibits a 10-fold, more preferably 100-fold, still more preferably 1000-fold and most preferably 10000-fold
5 higher solubility in water than the corresponding wild type, preferably human ligand-gated receptor. However, improvements in water solubility of about 2 to 5 fold is also already advantageous. The average hydrophobicity may be in the range of -100 to -400. Accordingly, the present invention provides methods for the prediction and creation of mutants and chimeras of ligand binding domains of homopentameric
10 acetylcholine receptor subtypes and of other homopentameric ion channels with increased solubility.

In one embodiment the water-soluble ligand-binding protein of the invention further comprises a spacer sequence allowing coupling with a carrier body. The spacer
15 sequence may be an amino acid sequence encodable by a polynucleotide or other molecule such as polymethylene anchor groups commonly used in chip technology. The chimeric protein of the invention may further comprise a spacer sequence, which allows coupling of the protein to a carrier body. Such spacer sequence may be e.g. an oligo-histidine stretch attached to the C-terminus of the protein. Such an oligo-
20 histidine stretch is capable of binding to Talon® metal affinity beads or similar carriers. Such binding stretches have no detectable influence on the pharmacological properties of the proteins. The chimeric proteins according to the invention can be used for screening of specific binding of potential drugs, in particular screening for modulators of ion-channel opening. Conventional in vitro screening techniques, such
25 as phage display technology, can be used for this purpose. High-throughput assays, possibly in combination with combinatorial chemistry can also be used. Specific binding of test compounds to the (immobilised) chimeric proteins of the invention can be performed e.g. by competition binding assays using alpha bungarotoxin as a competitor. The invention also concerns test kits containing the proteins described
30 above, together with further means for carrying out a screening test, such as carriers, labels, diluents, other chemicals etc.

In addition, the present invention relates to fusion proteins comprising the water-soluble ligand-binding protein of the invention or a binding fragment thereof and a
35 fragment of a ligand-gated receptor. The term "fusion protein" as used herein refers to protein constructs that are the result of combining multiple protein domains or linker regions for the purpose of gaining the combined functions of the domains or

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linker regions. This is may be accomplished by molecular cloning of the nucleotide sequences encoding such domains to produce a new polynucleotide sequence that encodes the desired fusion protein. Alternatively, creation of a fusion protein may be accomplished by chemically joining two proteins. A fusion protein of the present invention preferably comprises at least the ligand-binding domain of the AChBP or of a ligand-gated ion channel, which has been modified in accordance with the above described methods.

Nicotinic acetylcholine receptors are comprised of five subunits, selected from a related family of subunit proteins. The neuronal subunits fall into two main types depending on the presence or absence of a pair of vicinal cysteines close to the binding site for acetylcholine. Thus all α -subunits contain paired cysteine residues thought to play a role in binding of nicotinic agonists (Aplin and Wonnacott, 48 (1994), 473-477), whereas the β -subunits do not. There are ten known alpha subunits, $\alpha 1$ to $\alpha 10$, and at least four beta subunits, $\beta 1$ to $\beta 4$. Receptors comprise at least one alpha subunit which in some cell types combine with a beta subunit and in some cases a gamma, delta and epsilon subunit. For example, the AChR at the neuromuscular junction is believed to have an $(\alpha 1)2\beta 1\gamma\delta$ stoichiometry. Within the group of α -subunits there is marked diversity in the manner in which a complete functional nAChR is formed. The majority of the α subunits only form functional receptors when combined as a heteropentamer with β -subunits in the CNS (McGehee and Role, Annual Review of Physiology 57 (1995), 521-546). However, $\alpha 7$, $\alpha 8$ and $\alpha 9$ nAChR subunits and the related 5-HT3A subunit are capable of forming functional homopentameric receptors. In this respect it is interesting that the phylogenetic relationship between nAChR subunits suggest that $\alpha 7$, $\alpha 8$, $\alpha 9$ and the related 5-HT3A subunit are more related to each other than to the subunits which only form heteropentameric receptors. Sequence homologies indicate that the $\alpha 7$, $\alpha 8$ and $\alpha 9$ subunits form a distinct subgroup of the alpha subunits.

As is evident from the foregoing, the above described water-soluble ligand-binding protein or receptor or ligand-binding domain thereof can be used for forming complexes of homo- or heteromultimers, such as a dimer, pentamer or decamer consisting of at least one monomer of the mentioned proteins of the present invention. Preferably, these multimers constitute a function ligand-gated receptor. Preferably, said ligand-gated receptor is related to the nAChR.

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The present invention also relates to the production of synthetic heteropentamers resembling heteropentameric gated ion-channels by mutation of AChBP, using

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knowledge of the crystal structure about the primary and secondary contact regions; see *infra*. Preferably, said synthetic heteropentamer resembles a heteropentameric nicotinic acetylcholine receptor. Accordingly, the present invention more generally relates to a ligand-gated ion channel comprising any one of the above described

5 water-soluble ligand-binding proteins or receptors of the invention as a monomer, homo- or heterodimer or -pentamer. This method therefore allows the prediction and creation of mutants and chimeras of nicotinic acetylcholine receptors and other ligand-gated ion channels that are insensitive or more sensitive to toxin binding, e.g. bungarotoxin, lophotoxin, conotoxin, and other toxins that inhibit ligand-gated ion

10 channels. Preferably, said ligand-gated ion channel is less or more sensitive to binding of toxins such as bungarotoxin, lophotoxin or conotoxin compared to the wild type ligand-gated ion channel.

Further information and examples how to create chimeric ligand-binding proteins in accordance with the present invention is given in Example 10.

15

The nucleotide and amino acid sequences of the acetylcholine, 5-HT₃, glycine, GABA_A, and GABA_C receptors can be easily retrieved from public database, for example from the internet using <http://www.ncbi.nlm.nih.gov/Entrez>. The citations also include a reference to the corresponding publication also reporting on the

20 functional expression of the respective receptor.

The use of recombinant acetylcholine-gated ion channels and functional assays in the discovery of putative novel ligands has been described in Cosford, *Pharm. Acta Helv.* (2000), 74(2-3), 125-130. Furthermore, the cell-free expression and functional reconstitution of homo-oligomeric $\alpha 7$ nicotinic acetylcholine receptors into planar lipid

25 bilayers has been reported by Lyford and Rosenberg, *J. Biol. Chem.* (1999), 274(36), 25675-25681. The use of functional assays of cloned and native muscarinic acetylcholine receptors for determining the selectivity profile of toxins has been described by Olanas et al. (*J. Pharmacol. Exp. Ther.* 288 (1999), 164-170). A system for the evaluation of pharmacological differences and similarities between 5-HT₃

30 receptors stably transfected cells is provided by for example Bruss et al., *Naunyn-Schmiedeberg's Archives of Pharmacology* 360 (1999), 225-33. The primary structure and functional expression of the 5-HT₃ receptor is described in Maricq et al., *Science* 254 (1991), 432-437. Likewise, the stable expression of human glycine $\alpha 1$ and $\alpha 2$ receptor monomers in mouse L(tk-) cells and their use for the study of the physiology

35 and pharmacology of functional glycine receptors is described in Wick et al., *J. Neurosci. Methods* 87 (1999), 97-103. An example for the measurement of the

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pharmacology of recombinant GABA_A receptor subtypes is described in Simpson et al., J. Neurosci. Methods 99 (2000), 91-100. Further examples for assay systems are given below.

The described methods as well as others known to the person skilled in the art can be used for example to

- (1) express and characterise the water-soluble ligand-binding proteins and ligand-gated ion channels of the present invention; and
- (2) use stably transfected cells expressing the above described ligand-gated ion channels for the identification of novel ligands.

10

The present invention also relates to polynucleotides encoding the water-soluble ligand-binding proteins and ligand-gated ion channels of the present invention, and multimers thereof, preferably dimers or pentamers. Such polynucleotide may be a DNA such as a cDNA, or an RNA such as mRNA or any other form of nucleic acid including synthetic or modified derivatives and may encode the polypeptide in a continuous sequence or in a number of sequences interrupted by intervening sequences. In which ever form it is present, the polynucleotide is an isolated polynucleotide in that it is removed from its naturally-occurring state. This aspect of the invention is based on the cloning of the cDNA for ligand-binding proteins. In a preferred embodiment, the polynucleotide comprises the nucleotide sequence of any one of SEQ ID Nos. 1, 3, 5 or 7, optionally including one or more mutations or deletions which do not substantially affect the activity of the polypeptide encoded thereby. Such mutations include those arising from the degeneracy of the genetic code, as well as those giving rise to any of the amino acid mutations or deletions discussed above. The polynucleotides of the invention preferably comprise

25

- (a) a nucleotide sequence having at least 15 continuous nucleotides of the nucleotide sequence depicted in any one of SEQ ID Nos. 1, 3, 5 or 7 or a degenerated nucleotide sequence thereof; or
- (b) a nucleotide sequence capable of hybridizing to a nucleotide sequence of (a) under stringent hybridisation conditions.

30

Typically, selective hybridization will occur when there is at least about 55% sequence identity -- preferably at least about 65%, more preferably at least about 75%, and most preferably at least about 90% -- over a stretch of at least about 14 nucleotides; see, e.g., Kanehisa, Nucleic Acids Res. 12 (1984), 203-213, herein incorporated by reference. Nucleic acid hybridization will be affected by such conditions as salt concentration, temperature, solvents, the base composition of the

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hybridizing species, length of the complementary regions, and the number of nucleotide base mismatches between the hybridizing nucleic acids, as will be readily appreciated by those skilled in the art.

"Stringent hybridization conditions" and "stringent wash conditions" in the context of nucleic acid hybridization experiments depend upon a number of different physical parameters. The most important parameters include temperature of hybridization, base composition of the nucleic acids, salt concentration and length of the nucleic acid. One having ordinary skill in the art knows how to vary these parameters to achieve a particular stringency of hybridization. In general, "stringent hybridization" is performed at about 25°C below the thermal melting point (T_m) for the specific DNA hybrid under a particular set of conditions.

"Stringent washing" is performed at temperatures about 5°C lower than the T_m for the specific DNA hybrid under a particular set of conditions. The T_m is the temperature at which 50% of the target sequence hybridizes to a perfectly matched probe; see Sambrook et al., page 9.51, hereby incorporated by reference. The T_m for a particular DNA-DNA hybrid can be estimated by the formula:

$$T_m = 81.5^{\circ}\text{C} + 16.6 (\log_{10}[\text{Na}^+]) + 0.41 (\text{fraction G} + \text{C}) - 0.63 (\% \text{ formamide}) - (600/l)$$

where l is the length of the hybrid in base pairs.

The T_m for a particular RNA-RNA hybrid can be estimated by the formula:

$$T_m = 79.8^{\circ}\text{C} + 18.5 (\log_{10}[\text{Na}^+]) + 0.58 (\text{fraction G} + \text{C}) + 11.8 (\text{fraction G} + \text{C})^2 - 0.35 (\% \text{ formamide}) - (820/l).$$

The T_m for a particular RNA-DNA hybrid can be estimated by the formula:

$$T_m = 79.8^{\circ}\text{C} + 18.5 (\log_{10}[\text{Na}^+]) + 0.58 (\text{fraction G} + \text{C}) + 11.8 (\text{fraction G} + \text{C})^2 - 0.50 (\% \text{ formamide}) - (820/l).$$

In general, the T_m decreases by 1-1.5°C for each 1% of mismatch between two nucleic acid sequences. Thus, one having ordinary skill in the art can alter hybridization and/or washing conditions to obtain sequences that have higher or lower degrees of sequence identity to the target nucleic acid. For instance, to obtain hybridizing nucleic acids that contain up to 10% mismatch from the target nucleic acid sequence, 10-15°C would be subtracted from the calculated T_m of a perfectly matched hybrid, and then the hybridization and washing temperatures adjusted accordingly. Probe sequences may also hybridize specifically to duplex DNA under certain conditions to form triplex or other higher order DNA complexes. The preparation of such probes and suitable hybridization conditions are well known in the art. An example of stringent hybridization conditions for hybridization of complementary nucleic acid sequences having more than 100 complementary residues on a filter in a Southern or Northern blot or for screening a library is 50%

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formamide/6X SSC at 42°C for at least ten hours. Another example of stringent hybridization conditions is 6X SSC at 68°C for at least ten hours. An example of low stringency hybridization conditions for hybridization of complementary nucleic acid sequences having more than 100 complementary residues on a filter in a Southern or northern blot or for screening a library is 6X SSC at 42°C for at least ten hours. Hybridization conditions to identify nucleic acid sequences that are similar but not identical can be identified by experimentally changing the hybridization temperature from 68°C to 42°C while keeping the salt concentration constant (6X SSC), or keeping the hybridization temperature and salt concentration constant (e.g. 42°C and 6X SSC) and varying the formamide concentration from 50% to 0%. Hybridization buffers may also include blocking agents to lower background. These agents are well-known in the art; see Sambrook et al., pages 8.46 and 9.46-9.58, herein incorporated by reference. Wash conditions also can be altered to change stringency conditions. An example of stringent wash conditions is a 0.2x SSC wash at 65°C for 15 minutes (see Sambrook et al., for SSC buffer). Often the high stringency wash is preceded by a low stringency wash to remove excess probe. An exemplary medium stringency wash for duplex DNA of more than 100 base pairs is 1x SSC at 45°C for 15 minutes. An exemplary low stringency wash for such a duplex is 4x SSC at 40°C for 15 minutes. In general, signal-to-noise ratio of 2x or higher than that observed for an unrelated probe in the particular hybridization assay indicates detection of a specific hybridization.

By the provision of the nucleotide sequences of SEQ ID Nos. 1, 3, 5 and 7 as well as those encoding the amino acid sequences depicted in SEQ ID Nos. 2, 4, 6 and 8 it is possible to isolate identical or similar nucleic acid molecules which encode water-soluble ligand-binding proteins from other species or organisms, in particular orthologous water-soluble ligand-binding protein encoding genes from mammals. The term "orthologous" as used herein means homologous sequences in different species that arose from a common ancestor gene during speciation. Orthologous genes may or may not be responsible for a similar function; see, e.g., the glossary of the "Trends Guide to Bioinformatics", Trends Supplement 1998, Elsevier Science.

In a further aspect, the present invention provides a recombinant polynucleotide comprising a vector incorporating the polynucleotide of the present invention. Many suitable vectors are known to those skilled in molecular biology, the choice of which would depend on the function desired and include plasmids, cosmids, viruses, bacteriophages and other vectors used conventionally in genetic engineering. Methods which are well known to those skilled in the art can be used to construct

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various plasmids and vectors; see, for example, the techniques described in Sambrook, Molecular Cloning A Laboratory Manual, Cold Spring Harbor Laboratory (1989) N.Y. and Ausubel, Current Protocols in Molecular Biology, Green Publishing Associates and Wiley Interscience, N.Y. (1989), (1994). Alternatively, the polynucleotides and vectors of the invention can be reconstituted into liposomes for delivery to target cells. As discussed in further details below, a cloning vector was used to isolate individual sequences of DNA. Relevant sequences can be transferred into expression vectors where expression of a particular polypeptide is required. Typical cloning vectors include pBscpt sk, pGEM, pUC9, pBR322 and pGBT9. Typical expression vectors include pTRE, pCAL-n-EK, pESP-1, pOP13CAT, pET, pGEX, pMALC, pPIC9, pBac.

Hence, in a preferred embodiment of the present invention the above-described polynucleotides either alone or present in a vector are linked to control sequences which allow the expression of the polynucleotide in prokaryotic and/or eukaryotic cells.

The term "control sequence" refers to regulatory DNA sequences which are necessary to effect the expression of coding sequences to which they are ligated. The nature of such control sequences differs depending upon the host organism. In prokaryotes, control sequences generally include promotor, ribosomal binding site, and terminators. In eukaryotes generally control sequences include promoters, terminators and, in some instances, enhancers, transactivators or transcription factors. The term "control sequence" is intended to include, at a minimum, all components the presence of which are necessary for expression, and may also include additional advantageous components.

The term "operably linked" refers to a juxtaposition wherein the components so described are in a relationship permitting them to function in their intended manner. A control sequence "operably linked" to a coding sequence is ligated in such a way that expression of the coding sequence is achieved under conditions compatible with the control sequences. In case the control sequence is a promotor, it is obvious for a skilled person that double-stranded nucleic acid is preferably used.

Thus, the vector of the invention is preferably an expression vector. An "expression vector" is a construct that can be used to transform a selected host cell and provides for expression of a coding sequence in the selected host. Expression vectors can for instance be cloning vectors, binary vectors or integrating vectors. Expression comprises transcription of the nucleic acid molecule preferably into a translatable mRNA. Regulatory elements ensuring expression in prokaryotic and/or eukaryotic

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cells are well known to those skilled in the art. In the case of eukaryotic cells they comprise normally promoters ensuring initiation of transcription and optionally poly-A signals ensuring termination of transcription and stabilization of the transcript. Possible regulatory elements permitting expression in prokaryotic host cells

5 comprise, e.g., the PL, lac, trp, T7 or tac promotor in *E. coli*, and examples of regulatory elements permitting expression in eukaryotic host cells are the AOX1 or GAL1 promotor in yeast or the CMV-, SV40-, RSV-promotor (Rous sarcoma virus), CMV-enhancer, SV40-enhancer or a globin intron in mammalian and other animal cells. In this context, suitable expression vectors are known in the art such as

10 Okayama-Berg cDNA expression vector pcDV1 (Pharmacia), pCDM8, pRc/CMV, pcDNA1, pcDNA3 (In-vitrogene), pSPORT1 (GIBCO BRL). An alternative expression system which could be used to express the protein is an insect system. In one such system, *Autographa californica* nuclear polyhedrosis virus (AcNPV) is used as a vector to express foreign genes in *Spodoptera frugiperda* cells or in *Trichoplusia*

15 larvae. The coding sequence of a nucleic acid molecule of the invention may be cloned into a nonessential region of the virus, such as the polyhedrin gene, and placed under control of the polyhedrin promotor. Successful insertion of said coding sequence will render the polyhedrin gene inactive and produce recombinant virus lacking coat protein coat. The recombinant viruses are then used to infect *S.*

20 *frugiperda* cells or *Trichoplusia* larvae in which the protein of the invention is expressed (Smith, J. Virol. 46 (1983), 584; Engelhard, Proc. Nat. Acad. Sci. USA 91 (1994), 3224-3227).

In plants, promoters commonly used are the polyubiquitin promotor, and the actin promotor for ubiquitous expression. The termination signals usually employed are

25 from the Nopaline Synthase promotor or from the CAMV 35S promotor. A plant translational enhancer often used is the TMV omega sequences, the inclusion of an intron (Intron-1 from the Shrunk gene of maize, for example) has been shown to increase expression levels by up to 100-fold. (Mait, Transgenic Research 6 (1997), 143-156; Ni, Plant Journal 7 (1995), 661-676). Additional regulatory elements may

30 include transcriptional as well as translational enhancers. Advantageously, the above-described vectors of the invention comprises a selectable and/or scorable marker. Selectable marker genes useful for the selection of transformed cells and, e.g., plant tissue and plants are well known to those skilled in the art and comprise, for example, antimetabolite resistance as the basis of selection for dhfr, which

35 confers resistance to methotrexate (Reiss, Plant Physiol. (Life Sci. Adv.) 13 (1994), 143-149); npt, which confers resistance to the aminoglycosides neomycin,

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kanamycin and paromycin (Herrera-Estrella, EMBO J. 2 (1983), 987-995) and hygromycin, which confers resistance to hygromycin (Marsh, Gene 32 (1984), 481-485).

Useful scorable markers are also known to those skilled in the art and are commercially available. Advantageously, said marker is a gene encoding luciferase (Giacomin, Pl. Sci. 116 (1996), 59-72; Scikantha, J. Bact. 178 (1996), 121), green fluorescent protein (Gerdes, FEBS Lett. 389 (1996), 44-47) or β -glucuronidase (Jefferson, EMBO J. 6 (1987), 3901-3907). This embodiment is particularly useful for simple and rapid screening of cells, tissues and organisms containing a vector of the invention.

- 10 The proteins can be recovered and purified from recombinant cell cultures by well-known methods including ammonium sulfate or ethanol precipitation, acid extraction, anion or cation exchange chromatography, phosphocellulose chromatography, hydrophobic interaction chromatography, size exclusion chromatography, affinity chromatography, hydroxylapatite chromatography and lectin chromatography. Most
- 15 preferably, high performance liquid chromatography ("HPLC") or FPLC is employed for purification.

- The present invention furthermore relates to host cells produced by introducing a nucleic acid molecule into the host cell which upon its presence in the cell mediates
- 20 the expression of a gene encoding water-soluble ligand-binding proteins or comprising a polynucleotide or a vector as described above or a polynucleotide according to the invention wherein the polynucleotides and/or nucleic acid molecule is foreign to the host cell. By "foreign" it is meant that the polynucleotide or nucleic acid molecule is either heterologous with respect to the host cell, this means derived
- 25 from a cell or organism with a different genomic background, or is homologous with respect to the host cell but located in a different genomic environment than the naturally occurring counterpart of said nucleic acid molecule. This means that, if the nucleic acid molecule is homologous with respect to the host cell, it is not located in its natural location in the genome of said host cell, in particular it is surrounded by
- 30 different genes. In this case the polynucleotide may be either under the control of its own promotor or under the control of a heterologous promotor. The vector or nucleic acid molecule according to the invention which is present in the host cell may either be integrated into the genome of the host cell or it may be maintained in some form extrachromosomally. In this respect, it is also to be understood that the nucleic acid
- 35 molecule of the invention can be used to restore or create a mutant gene via homologous recombination.

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The host cell can be any prokaryotic or eukaryotic cell, such as bacterial, insect, fungal, plant or animal cells.

The term "prokaryotic" is meant to include all bacteria which can be transformed or transfected with a DNA or RNA molecules for the expression of a protein of the invention. Prokaryotic hosts may include gram negative as well as gram positive bacteria such as, for example, *E. coli*, *S. typhimurium*, *Serratia marcescens* and *Bacillus subtilis*. The term "eukaryotic" is meant to include yeast, higher plant, insect and preferably mammalian cells. Depending upon the host employed in a recombinant production procedure, the protein encoded by the polynucleotide of the present invention may be glycosylated or may be non-glycosylated. The water-soluble ligand-binding protein of the invention may or may not also include an initial methionine amino acid residue. A polynucleotide of the invention can be used to transform or transfect the host using any of the techniques commonly known to those of ordinary skill in the art. Furthermore, methods for preparing fused, operably linked genes and expressing them in, e.g., mammalian cells and bacteria are well-known in the art (Sambrook, *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Laboratory, Cold Spring Harbor, NY, 1989).

Thus the present invention provides a cell capable of expressing a polypeptide as discussed herein. The cell comprises a recombinant host cell usually incorporating the polynucleotide. Preferably, the host cell incorporates the polynucleotide as the recombinant polynucleotide. Any suitable host cell may be chosen, again depending on the intended purpose. Suitable host cells include XLI-BLUE, B21(DE3)pLysS, HB101, SOLR and SP-Q01 (*Saccharomyces pombe*).

Using an appropriate combination of host cell, vector and polynucleotide, an expression system can be provided so as to obtain a polypeptide useful in the present invention. This may comprise a fusion polypeptide encoded by the recombinant polynucleotide, a part of which is encoded by the vector. Typically, the vector will have a promotor region, which is usually inducible, leading to 5' coding region associated with the promotor. By appropriate manipulation, the polynucleotide encoding the polypeptide can be attached to the 5' coding region in frame. In this way, expression of the nucleotide sequence downstream of the promotor region gives rise to the fusion polypeptide which includes the polypeptide of the present invention.

The present invention also relates to an antigen comprising an epitope of at least 5 continuous amino acids of the amino acid sequence depicted in any one of SEQ ID Nos. 2, 4, 6 or 8 and/or said epitope is detectable by a monoclonal or polyclonal

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antibody which recognises, preferably with a binding affinity of at least $10^{-7}M$, a protein of the invention as described above. In the present invention, "epitopes" refers to fragments of the AChBP of the invention having antigenic or immunogenic activity in an animal. A preferred embodiment of the present invention relates to

5 antigens comprising an epitope, as well as the polynucleotide encoding this fragment. A region of a protein molecule to which an antibody can bind is defined as an "antigenic epitope." In contrast, an "immunogenic epitope" is defined as a part of a protein that elicits an antibody response; see, for instance, Geysen, Proc. Natl. Acad. Sci. USA 81 (1983); 3998-4002. Fragments which function as epitopes may be

10 produced by any conventional means; see, e.g., Houghten, Proc. Natl. Acad. Sci. USA 82 (1985), 5131-5135 further described in U.S. Patent No. 4,631,211. In the present invention, antigenic epitopes preferably contain a sequence of at least five, six, seven, more preferably at least nine, and most preferably between about 15 to about 30 amino acids. Antigenic epitopes are useful to raise antibodies, including

15 monoclonal antibodies, that specifically bind the epitope; see, for instance, Wilson, Cell 37 (1984), 767-778; Sutcliffe, Science 219 (1983), 660-666). Similarly, immunogenic epitopes can be used to induce antibodies according to methods well known in the art; see, for instance, Sutcliffe, supra; Wilson, supra; Chow, Proc. Natl. Acad. Sci. USA 82 (1985), 910-914; and Bittle, J. Gen. Virol. 66 (1985); 2347-2354.

20 A preferred immunogenic epitope includes the soluble protein. The immunogenic epitopes may be presented together with a carrier protein, such as an albumin, to an animal system (such as rabbit or mouse) or, if it is long enough (at least about 25 amino acids), without a carrier. However, Immunogenic epitopes comprising as few as 8 to 10 amino acids have been shown to be sufficient to raise antibodies capable

25 of binding to, at the very least, linear epitopes in a denatured polypeptide (e.g., in Western blotting.)

The present invention also relates to antibodies specifically recognizing the water-soluble ligand-binding protein and ligand-gated ion channels of the present invention,

30 In particular recognizing the above described antigen or epitope. As used herein, the term "antibody" (Ab) or "monoclonal antibody" (Mab) is meant to include intact molecules as well as antibody fragments (such as, for example, Fab and $F(ab)_2$ fragments) which are capable of specifically binding to protein. Fab and $F(ab)_2$ fragments lack the Fc fragment of intact antibody, clear more rapidly from the circulation, and may have less non-specific tissue binding than an intact antibody;

35 see, e.g., Wahl, J. Nucl. Med. 24 (1983), 316-325. Thus, these fragments are preferred, as well as the products of a FAB or other immunoglobulin expression

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library. Moreover, antibodies of the present invention include chimeric, single chain, and humanized antibodies; see also *infra*. Said antibody can be a monoclonal antibody, a polyclonal antibody, a single chain antibody, human or humanized antibody, primatized, chimerized or fragment thereof that specifically binds said peptide or polypeptide also including bispecific antibody, synthetic antibody, antibody fragment, such as Fab, Fv or scFv fragments etc., or a chemically modified derivative of any of these. The general methodology for producing antibodies is well-known and has been described in, for example, Köhler and Milstein, *Nature* 256 (1975), 494 and reviewed in J.G.R. Hurrel, ed., "Monoclonal Hybridoma Antibodies: Techniques and Applications", CRC Press Inc., Boca Raton, FL (1982), as well as that taught by L. T. Mimms et al., *Virology* 176 (1990), 604-619. Furthermore, antibodies or fragments thereof to the aforementioned peptides can be obtained by using methods which are described, e.g., in Harlow and Lane "Antibodies, A Laboratory Manual", CSH Press, Cold Spring Harbor, 1988. For the production of antibodies in experimental animals, various hosts including goats, rabbits, rats, mice, and others, may be immunized by injection with polypeptides of the present invention or any fragment or oligopeptide or derivative thereof which has immunogenic properties. Techniques for producing and processing polyclonal antibodies are known in the art and are described in, among others, Mayer and Walker, eds., "Immunochemical Methods in Cell and Molecular Biology", Academic Press, London (1987). Polyclonal antibodies also may be obtained from an animal, preferably a mammal, previously infected with the virus of the invention. Methods for purifying antibodies are known in the art and comprise, for example, immunoaffinity chromatography. Depending on the host species, various adjuvants or immunological carriers may be used to increase immunological responses. Such adjuvants include, but are not limited to, Freund's, complete or incomplete adjuvants, mineral gels such as aluminium hydroxide, and surface active substances such as lysolecithin, pluronic polyols, polyanions, peptides, oil emulsions and dinitrophenol. An example of a carrier, to which, for instance, a peptide of the invention may be coupled, is keyhole limpet hemocyanin (KLH). When derivatives of said antibodies are obtained by the phage display technique, surface plasmon resonance as employed in the BIAcore system can be used to increase the efficiency of phage antibodies which bind to an epitope of the peptide or polypeptide of the invention (Schier, *Human Antibodies Hybridomas* 7 (1996), 97-105; Malmberg, *J. Immunol. Methods* 183 (1995), 7-13). In many cases, the binding phenomena of antibodies to antigens is equivalent to other ligand/anti-ligand binding.

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In another embodiment the present invention relates to an oligonucleotide probe comprising a nucleotide sequence having at least 15 continuous nucleotides of a polynucleotide of the invention and/or encoding the above described antigen. Such oligonucleotides will usually specifically hybridize to a polynucleotide encoding a water-soluble ligand-binding protein of the invention. Specific hybridization occurs preferably under stringent conditions and implies no or very little cross-hybridization with nucleotide sequences encoding no or substantially different proteins. Such nucleic acid molecules may be used as probes and/or for the control of gene expression. Nucleic acid probe technology is well known to those skilled in the art who will readily appreciate that such probes may vary in length. Preferred are nucleic acid probes of 17 to 35 nucleotides in length. Of course, it may also be appropriate to use nucleic acids of up to 100 and more nucleotides in length. The nucleic acid probes of the invention are useful for various applications. On the one hand, they may be used as PCR primers for amplification of polynucleotides according to the invention. Another application is the use as a hybridization probe to identify polynucleotides hybridizing to the polynucleotides of the invention by homology screening of genomic DNA libraries. Nucleic acid molecules according to this preferred embodiment of the invention which are complementary to a polynucleotide as described above may also be used for repression of expression of a gene comprising such a polynucleotide, for example due to an antisense or triple helix effect or for the construction of appropriate ribozymes (see, e.g., EP-B1 0 291 533, EP-A1 0 321 201, EP-A2 0 360 257) which specifically cleave the (pre)-mRNA of a gene comprising a polynucleotide of the invention. Selection of appropriate target sites and corresponding ribozymes can be done as described for example in Steinecke, Ribozymes, Methods in Cell Biology 50, Galbraith et al. eds Academic Press, Inc. (1995), 449-460. Standard methods relating to antisense technology have also been described (Melani, Cancer Res. 51 (1991), 2897-2901). Said nucleic acid molecules may be chemically synthesized or transcribed by an appropriate vector containing a chimeric gene which allows for the transcription of said nucleic acid molecule in the cell. Such nucleic acid molecules may further contain ribozyme sequences as described above.

In this respect, it is also to be understood that the polynucleotide of the invention can be used for "gene targeting" and/or "gene replacement", for restoring a mutant gene or for creating a mutant gene via homologous recombination; see for example Mouellic, Proc. Natl. Acad. Sci. USA, 87 (1990), 4712-4716; Joyner, Gene Targeting, A Practical Approach, Oxford University Press.

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Furthermore, the person skilled in the art is well aware that it is also possible to label such a nucleic acid probe with an appropriate marker for specific applications, such as for the detection of the presence of a polynucleotide of the invention in a sample derived from an organism, in particular mammals, preferably human. A number of companies such as Pharmacia Biotech (Piscataway NJ), Promega (Madison WI), and US Biochemical Corp (Cleveland OH) supply commercial kits and protocols for these procedures. Suitable reporter molecules or labels include those radionuclides, enzymes, fluorescent, chemiluminescent, or chromogenic agents as well as substrates, cofactors, inhibitors, magnetic particles and the like. Patents teaching the use of such labels include US Patents US-A-3,817,837; US-A-3,850,752; US-A-3,939,350; US-A-3,996,345; US-A-4,227,437; US-A-4,275,149 and US-A-4,366,241. Also, recombinant immunoglobulins may be produced as shown in US-A-4,816,567 incorporated herein by reference.

Furthermore, the so-called "peptide nucleic acid" (PNA) technique can be used for the detection or inhibition of the expression of a polynucleotide of the invention. For example, the binding of PNAs to complementary as well as various single stranded RNA and DNA nucleic acid molecules can be systematically investigated using thermal denaturation and BIAcore surface-interaction techniques (Jensen, Biochemistry 36 (1997), 5072-5077).

The present invention also relates to a method for the production of a transgenic non-human animal, preferably transgenic mouse, comprising introduction of a polynucleotide or vector of the invention into a germ cell, an embryonic cell, stem cell or an egg or a cell derived therefrom. The non-human animal can be used in accordance with a screening method of the invention described herein. Production of transgenic embryos and screening of those can be performed, e.g., as described by A. L. Joyner Ed., Gene Targeting, A Practical Approach (1993), Oxford University Press. The DNA of the embryonal membranes of embryos can be analyzed using, e.g., Southern blots with an appropriate probe; see supra. The invention also relates to transgenic non-human animals such as transgenic mouse, rats, hamsters, dogs, monkeys, rabbits, pigs, C. elegans and fish such as Torpedo fish comprising a polynucleotide or vector of the invention or obtained by the method described above, preferably wherein said polynucleotide or vector is stably integrated into the genome of said non-human animal, preferably such that the presence of said polynucleotide or vector leads to the expression of the water-soluble protein of the present invention.

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The present invention further relates to composition comprising any one of the above described water-soluble ligand-binding proteins, multimers such as dimers or pentamers thereof, ligand-gated ion channels, polynucleotides, vectors, host cells, antigens, antibodies, or oligonucleotide probes of the invention; and optionally
5 suitable means for detection or performing a ligand-receptor binding assay. In this context, the present invention also relates to a method for identifying an agonist/activator or antagonist/inhibitor of a ligand-gated receptor comprising the steps of:

- 10 (a) contacting the water-soluble ligand-binding protein of the present invention, multimers such as dimers or pentamers thereof, or the ligand-gated ion channel of the invention or a cell expressing said protein in the presence of components capable of providing a detectable signal in response to ligand binding with a compound to be screened under conditions that permit binding of said compound to the ligand-binding protein; and
- 15 (b) detecting the presence or absence of a signal generated from the binding activity of the ligand-binding protein, wherein the presence/increase and absence/decrease of the signal is indicative for an agonist/activator and antagonist/inhibitor, respectively, of a ligand-gated receptor.

20 Since ligand-gated receptors are modulated allosterically by natural polyamines, such as spermine, and by polyamine derivatives, such as polyamine amides (e.g. philanthotoxin-343) and polymethylene tetraamines (e.g. methoctramine) (Usherwood, Farmaco. 55 (2000), 202-205) compounds comprising or based on such entities may be used as starting material for screening. An antagonist or agonist
25 that "modulates the activity" of a polypeptide and causes an altered signal, for example response in the cell refers to a compound that alters the activity of the protein so that it behaves differently in the presence of the compound than in the absence of the compound. Typically, the effect of an antagonist is observed as a blocking of agonist-induced receptor activation. Antagonists include competitive as
30 well as non-competitive antagonists. A competitive antagonist (or competitive blocker) interacts with or near the site specific for agonist binding. A non-competitive antagonist or blocker inactivates the function of the receptor by interacting with a site other than the agonist interaction site. As understood by those of skill in the art, bioassay methods for identifying compounds that modulate the activity of receptors
35 such as proteins of the invention generally require comparison to a control. One type of "control" is a cell or culture that is treated substantially the same as the test cell or test culture exposed to the compound, with the distinction that the "control" cell or

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culture is not exposed to the compound. For example, in methods that use voltage clamp electrophysiological procedures, the same cell can be tested in the presence or absence of compound, by merely changing the external solution bathing the cell. Accordingly, the response of the transfected cell to the "control" cell or culture to the same compound under the same reaction conditions. However, "control data" can also be used from the literature.

As described in Example 6 the 3-dimensional structure of AChBP could be solved by X-ray crystallography at 2.7Å resolution (current Rfactor = 27.9 %, Rfree = 30.0 %).

10 In crystals, as in solution, AChBP forms a stable homo-pentamer with dimensions comparable to those of the ligand-binding domain of ligand-gated ion channels, in particular comparable to the nAChR, as determined in EM studies by Unwin and coworkers; see supra. The structural analysis revealed that in the AChBP homopentamer the monomers have immunoglobulin-like topology. At each of five

15 subunit interfaces a ligand-binding site is located, with all residues consistent with biochemical data. In this site a buffer molecule (HERPES) stacks with cation- π interactions on a tryptophan, resembling acetylcholine binding. The AChBP structure is relevant for the development of drugs against, *e.g.*, Alzheimer's disease and nicotine addiction. The high-resolution crystal structure of AChBP, along with

20 biochemical and pharmacological data, supports the teaching of the present invention that the water-soluble ligand-binding proteins of the invention such as AChBP are good mimics of ligand-binding domains of ligand-gated ion channels.

Thus, the present invention relates to a crystal of a water-soluble ligand-binding protein of the invention, preferably in a multimeric form such as dimer, pentamer or

25 decamer. In one embodiment said crystal comprises a protein-ligand complex.

Methods how to employ and analyze such crystals are known to the person skilled in the art; see for example US-A-5,872,011 which describes the crystal structure of a protein-ligand complex containing an N-terminal truncated eIF4E and uses thereof.

30 The crystal structure of the ligand-gated receptor ligand-binding region in a complex with a ligand, preferably being an antagonist or agonist will reveal the determinants of receptor-antagonist/agonist interactions and how ligand-binding specificity and affinity are altered by remote residues and the redox state of the conserved disulphide bond. The structure may also indicate mechanisms for allosteric effector

35 action and for ligand-induced channel gating. How the information on the crystal structure of a ligand-binding region in a complex with a ligand can be used for the development of agonists and antagonists has been described for the structure of a

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glutamate-receptor ligand-binding core in complex with kainate (Armstrong et al., Nature 395 (1998), 913-917).

5 The crystal of the invention, in particular when comprising nAChR related proteins can be a complex of the protein with a ligand comprising an N-alkylated hydroxyalkyl and/or a quaternary ammonium ion. However, other ligands may be used as well. Preferred ligands comprise 4-(2-Hydroxyethyl)-1-piperazineethanesulfonic acid (HEPES), B-bippinatin, lophotoxin, d-tubocurarine, nicotine, acetylcholine, conotoxin, carbamylcholine, galanthamine, epibatidine or alpha-bungarotoxin or derivatives thereof.

10 Different aspects of X-ray crystallography are such as data collection, structure solution, determining the molecular structure from X-ray diffraction, refinement, etc. are described in the prior art, see, e.g., Powell, Annu. Rep. Prog. Chem., Sect. C: Phys. Chem. 96 (2000), 139-175 and Methods in Enzymology, 276-277, edited by Carter and Sweet, Academic Press, 1997. Current methods and optimization algorithms for the refinement of X-ray crystal structures are described by Van Der Maelen Uria, Crystallogr. Rev. 7 (1999), 125-180.

20 The crystal of the invention effectively diffracts X-rays for the determination of the atomic coordinates of the protein or protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms. In a preferred embodiment the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 3.0 Angstroms. In a more preferred embodiment the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 2.0 Angstroms. In one embodiment the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of about 2.7 Angstroms.

30 Preferably, the crystal of the invention is formed by a protein that has an amino acid sequence of amino acids 20 to 223 of SEQ ID No. 2, or an amino acid sequence that differs from amino acid 20 to 223 of SEQ ID No. 2 by only having conservative substitutions. As is described in the examples, the crystals of the AChBP comprise decameric forms of the protein. In order to ease the use of the AChBP protein for analysis and crystallography it is envisaged to create a mutation in residue Asp2 and Asp5 of the mature AChBP SEQ ID No. 2 or 4 to remove the calcium binding site, and prevent creation of a decamer. This deletion can be done for example by

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oligonucleotide-directed mutagenesis. Alternatively crystals could be grown in a low calcium concentration or in the absence of calcium.

5 The crystal of the present invention preferably has (1) a space group of $P2_12_12_1$ and a unit cell of dimensions of $a=120.6\text{\AA}$, $b=137.0\text{\AA}$ and $c=161.5\text{\AA}$; (2) a space group of $P4_22_12$ and a unit cell of dimensions of $a=b=141.6\text{\AA}$ and $c=120.8\text{\AA}$ or (3) a space group of $P2_1$ and a unit cell of dimensions of $a=121.1\text{\AA}$, $b=162.1\text{\AA}$, $c=139.4\text{\AA}$, $\beta=90.1^\circ$.

10 The crystal of the present invention is preferably from a protein that has secondary structural elements that include α -helix and antiparallel β -sheets as shown in and described for Figures 7, 10, 11 and/or 12. Most preferably, the crystal of the invention has a three-dimensional structure as defined by atomic coordinates shown in Table 1. Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of
15 this invention, any set of structure coordinates for AChBP or AChBP mutants that have a root mean square deviation of protein backbone atoms (N, C α , C and O) of less than 0.75 Angstrom when superimposed - using backbone atoms - on the structure coordinates listed in Table 1 shall be considered identical.

20 In a most preferred embodiment of the present invention, the crystal has a binding cavity as shown in Figures 6, 8, 9 and/or 13.

In accordance with the findings of the present invention, it is proposed to use the water-soluble ligand-binding proteins of molluscs as the blueprint for the receptor binding site of the ligand-gated ion channel superfamily including nACh, 5-HT₃, glycine, GABA_A, and GABA_C, most preferably for the nAChR. The availability of X-ray
25 structures, and the cloned sequences provide a unique opportunity to understand these receptors at the molecular level, possibly unravel the dynamic changes occurring upon ligand binding, and predict their tertiary and quaternary structure with a higher degree of confidence than possible for other protein modules. This should pave the way for designing ligands selective for any of the multiple subtypes in any of
30 these receptor families. The AChBP-like structures can be used for computerized docking to homology models which leads to the *a priori* discovery of novel ligands before laboratory experiments begin to optimize the drug candidates.

Thus, the present invention also relates to a method of using the crystal of the invention in a drug screening assays, such as comprising:

- 35 (a) selecting a potential ligand by performing structure assisted drug design with the three-dimensional structure determined for the crystal,

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wherein said selecting is performed in conjunction with computer modeling; optionally

- (b) contacting the potential ligand with the ligand binding domain of the ligand-gated receptor in an in vitro or in vivo assay; and
- 5 (c) detecting the binding of the potential ligand for the ligand binding domain.

The use of macromolecular crystallography as a tool for investigating drug and receptor interactions, in particular structure-based drug design is reviewed in Oakley
10 and Wilce, Clin. Exp. Pharmacol. Physiol. 27 (2000), 145-151. The desired drug could be an inhibitor or an agonist that mimics endogenous transmitters or ligands. Once the 3-D structure of the relevant target is known, computational processes can be used to search databases of compounds to identify ones that may interact strongly with the target. Lead compounds can be improved using the 3-D structure of
15 the complex of the lead compound and its biological target. The activity of the selected compound can then be tested in a functional assay such as one of those described herein..

Preferably, the potential drug is selected on the basis of its having a greater affinity for the ligand binding domain of the ligand-gated receptor than that of a standard
20 ligand for the ligand binding domain of the ligand-gated receptor. However, the affinity of the selected compound may also be less than that of a standard ligand. Such compounds are useful for example as a lead for the development of further analogues which in turn may have enhanced binding affinity or otherwise beneficial therapeutic properties. On the other hand, the selected compound may bind to a site
25 of the ligand-gated receptor other than known ligands. In a preferred embodiment, the ligand-gated receptor is a nicotinic acetylcholine receptor.

In a further embodiment, the method of the present invention further comprises:

- (d) forming a supplemental crystal of a protein-ligand complex by co-crystallization or soaking the crystal of the water-soluble ligand-binding
30 protein with a potential drug, wherein the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms, more preferably greater than 3;
- 35 (e) determining the three-dimensional structure of the supplemental crystal;

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- (f) selecting a candidate drug by performing a structure assisted drug design with the three-dimensional structure determined for the supplemental crystal, wherein said selecting is performed in conjunction with computer modeling; optionally
- 5 (g) contacting the candidate drug with a cell that expresses the ligand-gated receptor; and
- (h) detecting a cell response; wherein a candidate drug is identified as a drug when the cell response is altered compared to a cell that has not been contacted with the candidate compound.
- 10 The above described methods can further comprise an initial step that precedes step (a) wherein said initial step consists of determining the three-dimensional structure of a crystal comprising a protein-ligand complex formed between the water-soluble ligand-binding protein, and the ligand of the ligand-gated receptor, wherein the crystal effectively diffracts X-rays for the determination of the atomic coordinates of
- 15 the protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms. Preferably, the resolution of crystal diffraction in the above described methods is at least 3.0, most preferably at least about 2.7 Angstroms.

In a still further embodiment, the present invention relates to a method of growing a crystal of a protein-ligand complex comprising:

- 20 (a) contacting the water-soluble ligand-binding protein described above with a ligand of a ligand-gated receptor, wherein the water-soluble ligand-binding protein forms a protein-ligand complex with the ligand; and
- (b) growing the crystal of the protein-ligand complex; wherein the
- 25 crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms, more preferably at least 3.0, most preferably at least about 2.7 Angstroms.

- 30 The crystals of the present invention can also be used in X-ray crystallography-driven screening technique that combines the steps of lead identification, structural assessment, and optimization such as described for example in Nienaber et al., Nature Biotechnol. 18 (2000), 1105 - 1108. This crystallographic screening method (named CrystaLEAD) has been used to sample large compound libraries and
- 35 detecting ligands by monitoring changes in the electron density map of the crystal relative to the unbound form. The electron density map yields a high-resolution picture of the ligand-protein complex that provides key information to a structure-

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directed drug discovery process. The bound ligand is directly visualized in the electron density map. Ligands that bind away from the targeted site may be eliminated.

5 The above described methods can be coupled with state-of-the-art laboratory data collection facilities including CCD detectors and data acquisition robotics.

Further embodiments that may be used in accordance with the ligand-binding proteins and receptor of the present invention are described in the prior art, for example ligand screening and design by X-ray crystallography is disclosed in WO99/45379 and WO99/45389; WO00/14105 describes assaying a candidate
10 compound for its ability to interact with a modified receptor tyrosine kinase including obtaining and applying crystallography coordinates to a computer algorithm for generating a model which is applied in an iterative process to various molecular structures in order to identify agonist and antagonists of the receptor. All these methods may be equally applied to the proteins and crystals of the present invention.

15 In one preferred embodiment, the present invention relates to a drug screening assay comprising soaking a crystal of the invention in a solution of compounds to be screened and detecting the binding of the compound to the ligand-binding protein. A possible procedure is also described in Example 9. Besides the detection methods of
20 ligand-binding mentioned above, in the cited documents and in the examples, the detection can also be based on measuring the release of the ligand in the preformed crystal of a protein-ligand complex. As described herein before, said ligand preferably comprises an alkylated nitrogen and/or quaternary ammonium ion or may be one of those described above.

25 The structural information on the crystals of the present invention can also be used for increasing or decreasing the affinity of a drug to a ligand-gated receptor. Such a method can comprise performing structure assisted drug design with the three-dimensional structure determined for the crystal, wherein said drug design is
30 performed in conjunction with computer modeling; and modifying said drug to alter or eliminate a portion thereof suspected of interacting with a binding site of the binding cavity or with a non-specific binding site of the protein in the crystal. This method can, of course, be combined with one or more steps of any of the above described screening methods or other screening methods well known in the art. Methods for
35 clinical compound discovery comprises for example ultrahigh-throughput screening (Sundberg, Curr. Opin. Biotechnol. 11 (2000), 47-53) for lead identification, and structure-based drug design (Verlinde and Hol, Structure 2 (1994), 577-587) and

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combinatorial chemistry (Salemme et al., Structure 15 (1997), 319-324) for lead optimization. Further information that could be taken into account for drug selection and design so far available for the localization of agonist and competitive antagonist binding sites on nicotinic acetylcholine receptors have recently been reviewed (Arias, 5 Neurochem. Int. 36 (2000), 595-6450; Corringer et al., 1999). Once a drug has been selected, the method can have the additional step of repeating the method used to perform rational drug design using the modified drug and to assess whether said modified drug displays better affinity according to for example interaction/energy analysis.

10

A related method of the present invention for drug design comprises the step of using the structural coordinates of the water-soluble ligand-binding protein crystal comprising the coordinates of Table 1, to computationally evaluate a chemical entity for associating with the ligand-binding site or a non-specific binding site of a ligand-binding protein. This approach, made possible and enabled by this invention, is to 15 screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the AChBP. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, et al., J. Coma. Chem. 13 (1992), 505-524. In addition, in accordance with this invention, AChBP 20 mutants or chimerics may be crystallized in co-complex with known ligand-gated ion channel inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement (for review see for example Brunger et al. Prog. Biophys. Mol. Biol. 72 (1999), 135-155; and references cited therein) and compared 25 with that of wild-type AChBP. Potential sites for modification within the various binding sites of the ligand-binding domain may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between AChBP and a chemical entity or compound.

30 The design of compounds that bind to or inhibit ligand-gated ion channels according to this invention generally involves consideration of two factors.

First, the compound must be capable of physically and structurally associating with the ligand-binding domain. Non-covalent molecular interactions important in the association of the ligand-binding domain with its ligand include hydrogen bonding, 35 van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with the ligand-binding domain. Although certain portions of the compound

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will not directly participate in this association, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site or the spacing between functional groups of a compound comprising several chemical entities that directly interact with the AChBP.

If the theoretical structure of the given compound suggests insufficient interaction and association between it and AChBP, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to AChBP or a ligand-gated ion channel and functionally tested according to the methods mentioned above. In this manner, synthesis of inoperative compounds may be avoided. Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of AChBP. This would be followed by manual model building using software such as Quanta or Sybyl. Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include CAVEAT (Bartlett, et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In *Molecular Recognition in Chemical and Biological Problems*, Special Pub., Royal Chem. Soc. 78 (1989), 182-196); 3D Database systems such as MACCS-3D (Martin, J. Med. Chem. 35 (1992), 2145-2154) and HOOK (Molecular Simulations, Burlington, Mass.). Instead of proceeding to build an AChBP ligand in a step-wise fashion one fragment or chemical entity at a time as described above, AChBP binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known ligand(s). These methods include LUDI (Bohm, J. ComR. Aid. Molec. Design 6 (1992), 61-78); LEGEND (Nishibata and Itai, Tetrahedron 47 (1991), 8985); and LeapFrog (Tripos Associates, St. Louis, Mo.). Other molecular modelling techniques may also be employed in accordance with this invention; see, e.g., Cohen, J. Med. Chem. 33 (1990), 883-894 and Navia and Murcko, *Current Opinions in Structural Biology* 2 (1992), 202-210.

Such computer modeling is preferably performed with a Docking program (Dunbrack et al., *Protein Sci.* 6 (1997), 1661-1681 and *Folding Des.* 2 (1997), R27-R42).

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Methods for the identification of drugs or corresponding lead compounds in computational prescreen using X-ray crystal structures are described in the prior art

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(Verlinde and Hol, *Structure* 2 (1994), 577–587; Kuntz, *Science* 257 (1992), 1078–1082; Shuker et al., *Science* 274 (1996), 1531–1534; Fejzo et al., *Chem. Biol.* 6 (1999), 755–769; WO 98/58961). The structural information can be consulted to efficiently optimize leads. Computational programs have been written to identify compounds ranging from very small molecules or functional groups (GRID: Goodford, *J. Med. Chem.* 28 (1985), 849–857; MCSS: Caflish et al., *J. Med. Chem.* 36 (1993), 2142–2167) to potential lead scaffolds (DOCK: Kuntz et al., *Accounts Chem. Res.* 27 (1994), 117–123) using solved X-ray crystal structures. Another method computationally prescreens compound libraries and experimentally tests the individual "hits" by X-ray crystallography (Verlinde et al., *J. Comput. Aided Mol. Des.* 6 (1992), 131–147) in order to decrease the size of the screening library. In addition, an experimental approach has been developed to find organic solvents that bind to active sites that may be recombined into a lead macromolecule (Allen et al., *J. Phys. Chem.* 100 (1996), 2605–2611).

15

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to the AChBP or a corresponding ligand-binding domain may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as an inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. Inhibitors may interact with the ligand-binding domain in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the AChBP.

30

A compound designed or selected as binding to AChBP may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target ligand-binding domain. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the ligand and the AChBP when the ligand is bound to AChBP, preferably make a neutral or favorable contribution to the enthalpy of binding. Specific computer software is available in the art to evaluate compound deformation

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- energy and electrostatic interaction. Examples of programs designed for such uses include Gaussian 92, revision C (Frisch, Gaussian, Inc., Pittsburgh, Pa.); AMBER, version 4.0 (Kollman, University of California at San Francisco); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, Mass.); and Insight II/Discover (Biosym Technologies Inc., San Diego, Calif.). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS 4D/35, IBM RISC/6000 workstation model 550 or better a Unix workstation (SGI, Alpha, Sun, etc.) or any Linux PC. Other hardware systems and software packages will be known to those skilled in the art.
- Once an AChBP-binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to AChBP by the same computer methods described in detail, above. As mentioned before, the above described methods of the present invention can also be used as an initial drug screening assay followed by a classical drug screening assay using the biochemical assays known in the art.
- Methods for the preparation of compounds, chemical derivatives and analogues are well known to those skilled in the art and are described in, for example, Beilstein, Handbook of Organic Chemistry, Springer edition New York Inc., 175 Fifth Avenue, New York, N.Y.
- In one embodiment of the method of the present invention the identified drug prevents or promotes correct assembly of a ligand-gated ion channel. Thus, the selected drug may for example either interfere with the contact regions of the monomers of the ligand-gated ion channel or may act as a scaffold for the assembly.
- In the latter case, the drug may be based for example on an antibody which binds to the contact regions of two or more monomers when assembled and thus facilitates the assembly process. Preferred contact regions with respect to the AChBP and the related nicotinic acetylcholine receptor are given below. In a still further embodiment of the above described methods, the drug can be selected such as to bind to a non-specific binding site of a ligand-gated ion channel. The non-specific binding site can for example include those contact regions that are highly conserved between the monomers of the ligand-gated ion channels.

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Once a drug has been selected in accordance with any one of the above described methods of the present invention, the drug or a pro-drug thereof can be synthesized in a therapeutically effective amount. As used herein, the term "therapeutically effective amount" means the total amount of the drug or pro-drug that is sufficient to show a meaningful patient benefit, i.e., treatment, healing, prevention or amelioration of a condition related to an ligand-gated ion channel, or an increase in rate of treatment, healing, prevention or amelioration of such conditions. In addition or alternatively, in particular with respect to pre-clinical testing of the drug the term "therapeutically effective amount" includes the total amount of the drug or pro-drug that is sufficient to elicit a physiological response upon its binding to its target ligand-gated ion channel in an non-human animal test.

The present invention also relates to a drug produced by any one of the above described methods of the present invention, or a pro-drug thereof. Preferably, the drug or pro-drug thereof is present either alone or in a composition in a therapeutically effective amount.

The drug obtained by a method of the present invention may be characterized by its interaction with the binding sites in the binding cavity defined by the coordinates of crystal structure of the protein-ligand complex; for examples of such characterization see, e.g., US-A-5,798,247. Preferably, the drug, for example a potential inhibitor will form non-covalent bonds with one or more amino acids in the active site based upon the crystal structure. On the other hand, the drug may bind to a contact region of the individual monomers of the pentameric ligand-gated receptor. For example, multimer contact regions in *Lymnaea stagnalis* AChBP (SEQ ID No. 2) have been identified. Consecutive regions have at least every second residue involved in contacts with the other monomer. Contacts have been defined as 2 atoms within 4.2 angstrom distance in 2.7 Angstrom structure. The primary contact regions in mature AChBP (residues from A contacting B) are 15-21, 44-47, 85-87, 91-94, 122-124, 143-146, 149, 185-187 and the complementary contact regions (from B contacting A, (identical to residues on A contacting E) are 3-4, 7-8, 11, 37-39, 53, 75-77, 96-104, 114-118, 163-170; see also Figure 14.

Thus, in one preferred embodiment the drug of the present invention interacts with a ligand-gated receptor comprising a pentamer with monomers A to E, wherein the drug binds to one or more primary contact regions of a monomer (residues from A contacting B) defined by amino acid residues 15 to 21, 44 to 47, 85 to 87, 91 to 94, 122 to 124, 143 to 146, 149, 185 to 187 of SEQ ID No. 2 and/or to one or more of the

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complementary contact regions of the other monomer (from B contacting A, (identical to residues on A contacting E) defined by amino acid residues 3 to 4, 7 to 8, 11, 37 to 39, 53, 75 to 77, 96 to 104, 114 to 118 and 163-170 of SEQ ID No. 2; or to one of the contact regions identified in Figure 14; or to the corresponding contact regions of the monomers of a ligand-gated ion channel. Preferably, the ligand-gated ion channel is the nicotinic acetylcholine receptor and the order of the monomers is $\alpha\gamma\alpha\delta\beta$.

Any available method may be used to construct such model from the crystallographic and/or amino acid sequence data disclosed herein or obtained from independent analysis of crystalline AChBP proteins or other water-soluble ligand-binding proteins of the present invention. Such a model can be constructed from available analytical data points using known software packages such as HKL, MOSFILM, XDS, CCP4, SHARP, PHASES, HEAVY, XPLOR, TNT, NMRCOMPASS, NMRPIPE, DIANA, NMRDRAW, FELIX, VNMR, MADIGRAS, QUANTA, BUSTER, SOLVE, O, FRODO, RASMOL, CNS, REFMAC, ARP/WARP, XTALVIEW and CHAIN. The model constructed from these data can then be visualized using available systems, including, for example, Silicon Graphics, Evans and Sutherland, SUN, Hewlett Packard, Apple Macintosh, DEC, IBM, and Compaq. The present invention also provides for devices such as a computer system which comprises the model of the invention and hardware used for construction, processing and/or visualization of the model of the invention. Further embodiments provide a computer system comprising computer hardware and the model of the present invention. The study of the interaction of the candidate species with the model can be performed using available software platforms, including QUANTA, RASMOL, O, CHAIN, FRODO, INSIGHT, DOCK, MCSS/HOOK, CHARMM, LEAPFROG, CAVEAT (UC Berkley), CAVEAT (MSI), MODELLER, CATALYST, XTALVIEW and ISIS. Computer readable media such as floppy discs, CD ROMs, tapes, and any other storage or processing means comprising crystallographic and/or nucleotide/amino acid sequence data disclosed herein or obtained from independent analysis of crystalline AChBP proteins or other water-soluble ligand-binding proteins of the present invention are subject of the present invention as well. Any one of the mentioned means and devices can advantageously be used for modeling an antagonist/inhibitor or agonist/activator of a ligand-gated receptor.

Furthermore, the present invention relates to the construction of theoretical three dimensional (3D) models of ligand-binding domains of ligand-gated ion channels by computer-assisted molecular modeling using the X-ray coordinates of the water-soluble ligand-binding proteins of the invention. These 3D models can correspond

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either to the entire ligand-binding domain (~220 to 240 extracellular amino acids) or may be limited to the ligand-binding site.

The concept of using 3D structures of the mollusc ligand-binding proteins for molecular modeling and tool for structure prediction of for example mammalian, in particular human ligand-gated ion channels gains support from the observation that the ligand-binding domain of vertebrate glutamate receptor channels and bacterial periplasmic substrate-binding proteins (PBPs) share similar 3D structures despite the very low sequence similarity between ionotropic glutamate receptor subunits and the PBPs that were used as templates (12%); for review see Paas et al. *TIPS* 21 (2000), 87- 92 and references cited therein

Thus, on the basis of a computer-assisted molecular modeling, optionally supplemented by for example functional studies of site-specific mutants, the crystal structure of the ligand-binding domain of ligand-gated ion channels and theoretical 3D models of these domains can be predicted. In turn, these models can be used for structure assisted drug design. The predicted models may be further refined, for example by monitoring the effects of mutations of amino acid residues that are probably located in the ligand-binding site on (1) agonist-elicited channel activation and desensitization, (2) inhibition of channel activity by various competitive receptor antagonists; or (3) the binding of various ligands. Experimental setups for analyzing such effects are known to the person skilled in the art, see also the documents cited for functional assay systems of ligand-gated ion channels.

Thus, the embodiments of the present invention enable various possibilities for identification and modeling new ligands of ligand-gated ion channels as well as modifying the ion channels themselves. Accordingly, the present invention relates to the use of the above described polynucleotides, proteins, dimers and pentamers, ligand-gated ion channels, vectors, host cells, antigens, antibodies, oligonucleotide probes, crystals, their structural coordinates and methods for screening or profiling putative ligands of ligand-gated receptors.

Methods for the lead generation in drug discovery using proteins and detection methods such as mass spectrometry (Cheng et al. *J. Am. Chem. Soc.* 117 (1995), 8859-8860) and some nuclear magnetic resonance (NMR) methods (Fejzo et al., *Chem. Biol.* 6 (1999), 755-769; Lin et al., *J. Org. Chem.* 62 (1997), 8930-8931).

The newly identified drug obtained by a method of the present invention, i.e. an antagonist/inhibitor or agonist/activator can be used for the preparation of a pharmaceutical composition for the treatment of a ligand-gated ion channel mediated or related disorder. Such disorders are well known to the person skilled in the art. For

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example, possible applications of agonist and antagonists to nAChRs are based on their participation in complex functions such as attention, memory, and cognition, and their involvement in the pathogenesis of certain neuropsychiatric disorders (Alzheimer's and Parkinson's diseases, Tourette's syndrome, schizophrenia, depression, etc). For the majority of these disorders, the use of nAChRs' agonists may represent either a prophylactic (esp. for Alzheimer's and Parkinson's diseases) or a symptomatic treatment; for review see for example Mihailescu and Drucker-Colin, Arch. Med. Res. 31 (2000), 131-144.

The medicinal chemistry and molecular biology of GABA-activated ligand-gated ion channels also in terms of agonist and antagonist structural profiles is described in Chebib et al., J. Med. Chem. 43 (2000), 1427-1447.

Glycine receptors and disorders of glycinergic neurotransmission are extensively reviewed in Rajendra et al., Pharmacol. Ther. 73 (1997), 121-146 and Barry et al., Clin. Exp. Pharmacol. Physiol. 26 (1999), 935-936.

The central role of 5-HT₃ receptor in CNS disorders and 5-HT₃ receptor antagonists are described in Bloom and Morales, Neurochemical Research 23 (1998), 653-659 and Higgins and Kilpatrick, Expert Opin. Invest. Drugs 8 (1999), 2183-2188.

In one embodiment, the antagonist/inhibitor is or is derived from a protein, an antigen, antibody or from a toxin of the ligand-gated ion channel. Likewise, the agonist/activator can be derived from a protein, an antigen, antibody or from a toxin of the ligand-gated ion channel. Possible starting points comprise for example peptide toxins, e.g., conotoxin (IMI) and alpha bungarotoxin, lophotoxins (Bippinatsins), tubocurarine, decamethonium, alpha-cobratoxin, epibatidine, acetylcholine, choline, nicotine, carbachol, serotonin or GABA. The structure of these molecules together with that of the crystal of the target ligand-binding domain can be used to model the compound and elucidate side chains, functional groups etc. which may be added, deleted or modified in order to improve for example affinity and/or specificity of the drug or for example make a drug which acts on a different target non-reactive with a certain ligand-gated ion channel.

In a preferred embodiment for the uses according to the present invention, the ligand-gated ion channel is the nicotinic acetylcholine receptor and said mediated or related disorder is Tourette's syndrome, Alzheimer's disease, addiction to nicotine or schizophrenia.

As mentioned herein before, this is the first time it could be shown that water-soluble ligand-binding proteins exists in molluscs, which closely resemble the ligand-binding

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domain of ligand-gated ion channel of higher mammals. It is expected that similar ligand-binding proteins exist in other molluscan species or even in the lineage the Mollusca, Protostomia, Coelomata, Bilateria, Eumetazoa, Metazoa, Fungi/Metazoa group. Accordingly, the present invention also relates to the use of a ligand of a

5 ligand-gated ion channel for identifying and isolating a water-soluble ligand-binding protein from such species, preferably from a mollusc. Preferably, the ligand used for the isolation of the protein is α -bungarotoxin. The water-soluble ligand binding proteins obtainable from these organisms as well as derivatives that can be made in accordance with the teaching present herein are also subject of the present

10 invention.

Furthermore, for the first time the crystal structure of a nicotinic binding site has been revealed. This crystal structure shows that the molluscan AChBP is a homolog of the LGIC superfamily ligand binding domains. It reveals the Ig-topology, the location of

15 the binding site at the subunit interface, the position of the MIR and the extensive data on the nicotinic ligand binding residues. Importantly, it gives important new information about the exact fold and the arrangement of the nicotinic ligand-binding site in three dimensions. It shows the presence of a second pocket that has been noticed by EM analysis. Furthermore, it clarifies the arrangement of subunits by

20 showing the relative positioning of the principal and complementary part of the ligand-binding site. It provides an explanation of the role of the LGIC superfamily conserved residues in stabilizing the monomer structure by the formation of hydrophobic cores and packing of secondary structure elements and it makes clear how the pentamers are built up, and how weakly the pentamer interfaces are

25 conserved between LGICs.

This structure can be used for the numerous drug-design studies that are targeting the LGIC superfamily. The general structural knowledge on its folding will be applicable to the GABA, serotonin (5HT₃) and glycine receptor fields. It will help to understand their ligand-binding characteristics and could thus have impact on

30 development of *e.g.* anti-emetics aimed at the 5HT₃ receptor or the mood-defining drugs that target the GABA receptors. However, the availability of a three-dimensional description of the nicotinic ligand-binding site will be especially relevant for the design of new drugs against Alzheimers' disease, epilepsy and the addiction to smoking which have the neuronal nicotinic receptors as their targets.

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Many embodiments and the examples feature the acetylcholine-binding protein (AChBP) of the invention and the embodiments generally described herein are

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preferably related to the nicotinic acetylcholine receptor (nAChR), more preferably to the alpha subunit, and most preferably to the alpha 7 subunit. However, it should be understood that all embodiments equally apply to the other water-soluble ligand-binding proteins and generally to the ligand-gated ion channels mentioned herein.

- 5 For example, the crystal structure of the AChBP can be used to model new ligands for the acetylcholine receptor, preferably such with inhibiting or stimulating action on the acetylcholine receptor. Likewise, it is possible to identify and model new ligands for other ligand-gated ion channels (including glycine, GABA and serotonin receptor) with inhibiting action. Such ligands may for example prevent correct assembly of
- 10 ligand gated ion channels. Preferably such ligands prevent correct assembly of specific sub types of ligand gated ion channels. On the other hand, ligands can be identified and modeled that promote correct assembly of ligand gated ion channels, preferably of specific sub types of ligand gated ion channels. As mentioned before, the methods of the present invention also allow modelling inhibitors for the non-
- 15 specific binding site of ligand gated ion channels.

- In addition, it is possible to predict and create mutants and chimeras of AChBP with modified assembly behaviour, modified ligand binding behavior such as with increased resemblance of the binding site to the acetylcholine receptor subtype on the primary binding site and generally with increased resemblance to particular
- 20 ligand-gated ion channels in activity and conformational changes. In view of the closest relationship between AChBP and the acetylcholine receptor it is particular preferred to create mutants and chimeras with increased resemblance of the binding site to the acetylcholine receptor subtype on the secondary binding site. However, the prediction and creation of mutants and chimeras with increased resemblance of
- 25 the binding site to other ligand gated ion channels subtype on the primary binding site or on the secondary binding site are envisaged as well.

- These and other embodiments are disclosed and encompassed by the description and Examples of the present invention. Further literature concerning any one of the
- 30 antibodies, methods, uses and compounds to be employed in accordance with the present invention may be retrieved from public libraries and databases, using for example electronic devices. For example the public database "Medline" may be utilized which is available on the Internet, for example under <http://www.ncbi.nlm.nih.gov/PubMed/medline.html>. Further databases and
- 35 addresses, such as <http://www.ncbi.nlm.nih.gov/>, <http://www.infobiogen.fr/>, http://www.fmi.ch/biology/research_tools.html, <http://www.tigr.org/>, are known to the person skilled in the art and can also be obtained using, e.g., <http://www.lycos.com>.

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An overview of patent information in biotechnology and a survey of relevant sources of patent information useful for retrospective searching and for current awareness is given in Berks, TIBTECH 12 (1994), 352-364.

- 5 This disclosure may best be understood in conjunction with the accompanying drawings, incorporated herein by references. Furthermore, a better understanding of the present invention and of its many advantages will be had from the following examples, given by way of illustration and which are not intended as limiting.
- 10 Unless stated otherwise in the examples, all recombinant DNA techniques are performed according to protocols as described in Sambrook et al. (1989), Molecular Cloning : A Laboratory Manual. Cold Spring Harbor Laboratory Press, NY or in Volumes 1 and 2 of Ausubel et al. (1994), Current Protocols in Molecular Biology, Current Protocols. Standard materials and methods for plant molecular work are
- 15 described in Plant Molecular Biology Labfax (1993) by R.D.D. Croy, jointly published by BIOS Scientific Publications Ltd (UK) and Blackwell Scientific Publications (UK).

20 **Brief description of the drawings**

Figure 1: Clustal X (1.8) multiple sequence alignment of AChBP amino acid sequences. The AChBP alignment was made using "ClustalX_1.8" (Thompson et al., Nucleic Acids Research 24 (1997), 4876-4882. The

25 subsequent alignment was further processed using "Genedoc" version 2.5.000 (Nicholas et al. (1997) Genedoc a tool for editing and annotating multiple sequence alignments). Identical amino acids are indicated with "***", equivalent amino acid with ":", and similar amino acids with ".". Glycosylation sites are Asn 66 for L-AChBP and Asn 21 and 26 for B-AChBP in the amino acid sequence of the respective

30 mature AChBP SEQ ID No. 2 and 4, and 6 and 8, respectively.

Figure 2: Hydrophobicity plots of the mature AChBP amino acid sequences. The B&L-AChBP hydrophobicity plots were made using "Protein sequence analyses" according to the method described in Kyte and Doolittle (J. Mol. Biol. 157 (1982), 105-132). **2A:** L-AChBP_T1 (SEQ ID No. 2), **2B:** L-AChBP_T2 (SEQ ID No. 4), **2C:** B-AChBP_T1 (SEQ ID No. 6), **2D:** B-AChBP_T2 (SEQ ID No. 8).

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- Figure 3:** Clustal X (1.8) multiple sequence alignment of AChBP amino acid sequences with the amino acid sequences of the ligand-binding domains of the ligand-gated receptors nAChR- α 7, GABA_AR- β 1, 5-HT3R and GlyR- α 1. Sequence alignment and processing was performed as described for Figure 1. The accession numbers of the amino acid sequences used for the alignment are as follows: Human alpha1: Human alpha7: Y08420; Human 5HT3: CAA06442; Human GlyR_alpha1: S12382; Human GABA_A_b1: NP_000797. A similar sequence alignment can be performed with the corresponding rat sequences (ratnAChRa7_Q05941, rat5HT3R_P35563, ratGABARb1_P15431, ratGlyRa1_p24524) which will give substantially similar if not identical results.
- Figure 4:** Clustal X (1.8) multiple sequence alignment of AChBP amino acid sequences with the amino acid sequences of nAChRs. Sequence alignment and processing was performed as described for Figure 1. The accession numbers of the amino acid sequences used for the alignment are as follows: Human alpha1: ACHUA1; Human alpha2: AAG23253; Human alpha3: A53956; Human alpha4: P43681; Human alpha5: P30532; Human alpha6: Q15825; Human alpha7: Y08420; Human alpha9: CAB65091. A similar sequence alignment can be performed with the corresponding rat sequences (ratnAChRa7_Q05941, rnAChRa9_P43144, rnAChR2_P1238, rnAChRa3_P04757, rnAChRa4_P09483) which will give substantially similar if not identical results.
- Figure 5:** Clustal X (1.8) multiple sequence alignment of AChBP amino acid sequences with the amino acid sequences of nAChRs alpha 1 and 7. Sequence alignment and processing was performed as described for Figure 1. The accession numbers of the amino acid sequences used for the alignment are as follows: Human alpha1: ACHUA1; Human alpha7: Y08420. A similar sequence alignment can be performed with

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the corresponding rat sequence ratnAChRa7_Q05941 which will give substantially similar if not identical results.

5 **Figure 6:** The pentameric structure of AChBP. **a** In this schematic representation
each monomer has a different grey level. Subunits are labeled anti-
clockwise, with A-B, B-C, C-D, D-E and E-A forming the plus and
minus interface side, with the principal and complementary ligand-
binding sites respectively (ball-and-stick representation). **b** Viewing the
10 AChBP pentamer perpendicular to the five-fold axis. The equatorially
located ligand-binding site (ball-and-stick representation) is highlighted
only in the A (light) and B (dark) interface.

15 **Figure 7:** The AChBP monomer. Ribbon representation of the AChBP monomer.
The secondary structure starting from the N-terminus (top) towards the
C-terminus (bottom). The monomer is viewed towards the center of
the pentamer. In the nAChR, the top would correspond to the N-
terminus of the ligand binding domain, pointing towards the synaptic
cleft, while the C-terminus would be entering the membrane at the
20 bottom, continuing into the transmembrane domain. The AChBP
monomer is built up mainly of β -strands, except for an N-terminal α -
helix. It contains 14 β -strands that are organized in the two antiparallel
 β -sheets, with an immunoglobulin topology. However, in contrast to
the classical immunoglobulin fold, the AChBP β -sheets are rotated
25 against each other, forming a small pocket, as visible in Figure 6.

30 **Figure 8:** The ligand-binding site at dimer interface. Ribbon representation of
two neighboring AChBP monomers. Monomer A is shown in grey and
monomer B in dark grey. The ligand-binding site is located at the
interface between two monomers. As predicted for the nAChRs, the
acetylcholine binding site in AChBP occurs at the interface between
two neighboring subunits. Similar to the model proposed for the
nAChRs, the ligand-binding site is asymmetric, formed mainly by
aromatic residues. Residues from mature AChBP monomer A
35 (TyrA89, TrpA143, TyrA185, CysA187, CysA188 and TyrA192) form
the principal component, while residue TrpB53 from monomer B

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creates the complementary part of the ligand-binding site. There are five identical ligand-binding sites in the AChBP pentamer, similar to the homomeric $\alpha 7$ neuronal receptor.

- 5 **Figure 9:** The ligand binding site. Stereo figure showing the ligand binding site in AChBP, at the interface of two monomers. Residues from mature AChBP monomer A (TyrA89, TrpA143, TyrA185, CysA187, CysA188 and TyrA192) form the principal component, while residue TrpB53 from monomer B creates the complementary part of the ligand-binding site with with additional residues ArgB104, LeuB112 and MetB114. There are five identical ligand-binding sites in the AChBP pentamer, similar to the homomeric $\alpha 7$ neuronal receptor.
- 10
- 15 **Figure 10:** Multiple sequence alignment of AChBP amino acid sequences with indication of secondary structure and solvent accessibility derived from the crystal structure. Alignment of the four molluscan AChBP sequences, with secondary structure and solvent accessibility of the *Lymnea stagnalis* AChBP-1 indicated from the crystal structure. The Figure was prepared with ESPript (Gouet et al., Bioinformatics. 15 (1999), 305-308), using DSSP (Kabsch and Sander, Biopolymers. 22 (1983), 2577-2637). Under the alignment the solvent accessibility is indicated, white most buried, dark blue most exposed, according to ESPript defaults (blue $A > 0.4$, cyan $0.1 < A < 0.4$, white $A < 0.1$).
- 20
- 25 **Figure 11:** Sequence alignment of AChBP with LGICs. The alignment shows only the N-terminal domain of the LGIC subunits and is based on a multi-sequence alignment of 92 full-length LGIC sequences. Abbreviations used, H and Tca, stand for human and *Torpedo californica*. Secondary structure elements (α : α -helix, β : β -strand, η : 3_{10} -helix) are indicated above the sequence, in accordance with Fig 12a. AChBP shares 23% sequence identity with the ligand-binding domain of human $\alpha 7$. The LGIC conserved residues (bold, grey background) are displayed. Beginning and end of the Cys-loop are indicated by a "***". Nicotinic receptor ligand-binding residues on the principal and complementary side are indicated.
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Figure 12: Overview of the AChBP monomer structure. **a** Stereo representation of the AChBP monomer as viewed from outside the pentameric ring. Disulfide bridges are indicated in ball-and-stick representation. In a complete ion-channel the N-terminus would be pointing towards the synaptic cleft, while the C-terminus would enter the membrane at the bottom, continuing into the first transmembrane domain. **b** Topology diagram of the AChBP monomer. For comparison with Ig-folds the strands have been labeled a-g, showing the additional strand (b') and hairpin (f'-f''). In this structure, strands have been labeled $\beta 1$ - $\beta 10$ with loops (or turns) L1-L10 preceding each strand with the same number. The $\beta 5$ strand is broken ($\beta 5$ - $\beta 5'$) with internal loop L5', $\beta 6$ also has a small break, but is shown continuously; (see Fig. 11). The precise beginnings and ends of strands may change slightly with increasing resolution, but the topology seen here will be highly conserved across the entire family of LGICs.

Figure 13: The ligand-binding site. **a** Stereo representation of the ligand-binding site in ball-and-stick representation, showing the contribution of the principal A (TyrA89/ α_1 Tyr93), B (TrpA143/ α_1 Trp149) and C (TyrA185/ α_1 Tyr190, CysA187/ α_1 Cys192, CysA188/ α_1 Cys193, TyrA192/ α_1 Tyr198) and the complementary D (TrpB53/ γ Trp55, GlnB55/ γ Glu57), E (ArgB104/ γ Leu109, ValB106/ γ Tyr111, LeuB112/ γ Tyr117, MetB114/ γ Leu119) and F (TyrB164) 'loops'. **b** Stereo view of the electron density map displaying a HEPES buffer molecule in the ligand-binding site. This experimental density (contoured at 1 σ) is derived from cross-crystal averaging. **c** Location of the principal ligand-binding residues on the monomer. **d** Location of the complementary ligand-binding residues on the monomer. (orientation as in Figure 6b)

Figure 14: Dimer interface **a** Stereo figure of the dimer interface. Representation of the interface residues (ball-and-stick) on a schematic secondary structure figure. The figure shows the plus face of subunit A and the minus minus face of subunit B **b** Dimer interface interactions. Note that due to the low conservation of these interfaces (Fig. 11) the actual interactions will not be conserved in any LGIC interface, but that in all receptors the topological regions are likely to form the interface.

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Figure 15: Conservation in the LGIC superfamily. Conserved residues are indicated on the top, middle and bottom respectively on the monomer as viewed from the central pore. The hydrophilic conserved residues are indicated in dark. Conserved residues are indicated as viewed from the central pore. Hydrophobic Cluster I: residues 6, 10, 63, 65, 71, 81, 105, 111; Cluster II: residues 20, 27, 29, 31, 58, 82, 84, 86, 140, 150, 152, 195; Cluster III: residues 33, 35, 38, 41, 48, 52, 125, 138, 171, 173, 199, 201. The hydrophilic conserved residues: Asp60, Asp85, Asn90, Gly109, Cys123, Cys136, Lys203. Conserved residues in the ligand binding site: 106, 145, 192. These three and Lys203 are the only conserved residues without structural role in the monomer. Note how very few conserved residues are at the surface. Within the LGIC family the Cys-loop residues are also highly conserved; see bottom, left.

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EXAMPLES

EXAMPLE 1: Isolation of Lymnaea AChBP from the CNS, determination of mass and N-terminal protein sequence

Isolation: 80 CNS of *Lymnaea* were homogenized in lysis buffer (PBS [16 mM Na₂HPO₄, 4 mM NaH₂PO₄, pH 7.4; 150 mM NaCl] 0.5% Nonidet P-40; 0.1% triton, 0.2% tween-20) containing 1 ug/ml aprotinin, 10 ug/ml benzamidine, 0.5 ug/ml leupeptin, 24 ug/ml pefabloc. The CNS lysate was cleared by triplicate centrifugation at 12,000x g for 5 min. Streptavidin-coated magnetic beads (Dynal, Oslo), 5 mg, were saturated with α -bungarotoxin conjugated to Biotin (4 ug) (Molecular Probes, Oxford, UK). These beads were washed in PBS to remove excess α -bungarotoxin, then added to the cleared CNS lysate, and incubated for 1 h. After this, beads were washed 3 times in PBS to remove unbound protein. A control reaction without α -bungarotoxin was performed. Proteins bound to α -bungarotoxin were allowed to elute off in 10 μ l of PBS containing 10⁻⁴ M nicotine for 1h.

Mass determination: The eluent was separated on a microcolumn LC system was similar to that described previously (Hsieh et al.; Anal. Chem. 70; 1998; 1847-1852). A commercial syringe pump (Perkin-Elmer /ABI, model 140B) was used to deliver a flow rate of 20 μ l /min to the column. After loading of sample to the column the flow rate was dropped to 10 μ l /min. The eluent was then switched from 0.2% acetic acid to 0.2% acetic acid/ 60% acetonitril in 1 min. Electrospray mass spectra in MS mode were acquired on a Micromass Q-TOF quadrupole time-of-flight mass spectrometer equipped with a Z-spray atmospheric pressure ionization source.

25 Protein sequence analysis: For sequence analysis α -bungarotoxin binding protein was extracted using the same procedure, now followed by SDS-PAGE and Western Blotting on PDVF membrane. Sequence analysis was performed with Edman degradation of the 24 kDa blotted protein (apparent MW) using a protein sequencer (ABI, Perkin Elmer).

EXAMPLE 2: Cloning the *Lymnaea* AChBP cDNA sequence: PCR and screening of a cDNA library

PCR cloning: A degenerate oligonucleotide was synthesized based on the amino acid sequence LDRADILYNI (SEQ ID No. 10), residues 1-10, of AChBP, (5'-CGGATCCGA(TC)(AC)GIGC(GATC)GA(TC)AT(ATC)(TC)T(GATC)TA(TC)AA(TC)A T-3'; SEQ ID No. 11), containing a BamHI restriction site, and used in combination with a primer on the IZAPII lambda vector. PCR was performed on a IZAP II cDNA

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library of the *Lymnaea* CNS, in a 100 µl reaction volume with 1.0 unit of Super Taq DNA polymerase (Boehringer Mannheim, Germany) in a DNA thermal cycler (Perkin-Elmer Cetus, CT) using 45 cycles of (94 °C, 20 sec; 53 °C, 30 sec; and 72 °C, 1 min. Amplified cDNA was digested with *Bam*HI and *Eco*RI, separated on agarose gel, and a product of ~900 bp was cloned and sequenced.

Library screening: Approximately 20,000 clones of the amplified lambda ZAP II CNS cDNA library were plated at a density of 10⁵ pfu/400 cm² and absorbed to charged Nylon membranes (Boehringer Mannheim, Germany). The AChBP PCR product was used as a random primed probe, labeled with [α -³²P]dATP (specific activity >10⁹ cpm/mg). Membranes were hybridized in 6x SSC (1x SSC: 0.15 M NaCl and 0.015 M Na-citrate), 0.2% SDS, 5x Denhardtts and 10 µg/ml herring sperm DNA at 65 °C for 18 h. The filters were washed in 0.2x SSC, 0.2% SDS, at 65 °C for 30 min, and autoradiographed. Four individual cDNA clones were *in vivo* excised, and sequenced using dideoxy chain termination in both orientations. Two types of sequence were obtained, named L-AChBP_T1 and L-AChBP_T2. The signal sequences were determined with "SMART", Simple Modular Architectur Research Tool (V3.1); see Schultz et al., Proc. natl. Acad. Sci. USA 95 (1998), 5857-5864 and Nucleic Acids Res. 28 (2000), 231-234. In case of L-AChBP_T1 (SEQ ID No. 2) the prediction could experimentally be confirmed.

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EXAMPLE 3: *Lymnaea* AChBP-related sequences: cloning of the *Bulinus truncatus* cDNAs

Total RNA was isolated from *Bulinus* brain ganglia (CNS), and reverse transcribed into hexanucleotide primed cDNA. Two degenerate oligonucleotides, directed to the *Lymnaea* AChBP_T1 sequence, forward primer: 5'-GCGAATTCGAYACIGARWSIGGNGCNACNTG-3' (SEQ ID No. 12), reverse primer: 5'-GCGAAGCTTCRTCCTCCTAIGCYTCNGCRCARC-3' (SEQ ID No. 13), were used to amplify AChBP-related sequences. PCR was performed on one animal equivalent of CNS cDNA using 150 pmole of each primer under standard conditions for 45 cycles (94 °C, 20 sec; 54 °C, 30 sec; 72 °C, 1 min). Amplified cDNA was *Eco*RI/*Hind*III digested, cloned into *Eco*RI/*Hind*III digested pBluescript, and sequenced. The ORFs of the obtained sequences showed a *Bulinus* AChBP, sequence-related to *Lymnaea* AChBP, named B-AChBP_T1. This partial cDNA was used to screen a *Bulinus* brain cDNA library using the same hybridization protocol as described for the cloning of the *Lymnaea* cDNAs, and yielded two cDNA clones, encoding B-AChBP_T1 and B-AChBP_T2. Sequencing of the cDNAs was performed in both orientations.

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**EXAMPLE 4: The production of L-AChBP-T1 and -T2 and B-AChBP-T1 and -T2
in the yeast *Pichia pastoris* and functional characterization**

5 Production of recombinant AChBP:

In order to produce L-AChBP_T1 and T2 and B-AChBP_T1 and T2 as recombinant proteins in the *Pichia pastoris* expression system (*Pichia* Expression Kit version 3.0, Invitrogen), the DNA sequence encoding the mature form of these proteins (see sequence files) was cloned into the pPIC9 expression vector (Invitrogen). The mature sequences of L-AChBP_T1, T2 and B-AChBP_T1 and T2 were PCR amplified (using Pfu-taq DNA polymerase (Stratagene) in order to avoid introduction of errors into the sequence due to PCR) and restriction sites were added to the primers to allow rapid pPIC9 compatible cloning. The amplified sequence of mature AChBP L-AChBP_T1 was EcoRI inserted into pPIC9, whereas L-AChBP_T2 and B-AChBP_T1 and T2 were XhoI/EcoRI inserted into pPIC9 (the alpha-mating factor cleavage site was fully reconstructed after XhoI digestion).

Constructs with and without an additional C-terminal His-tag (SRGHHHHHH (SEQ ID No. 14) in the case of L-AChBP_T1, EFKDDDDKHHHHHH (SEQ ID No. 15) otherwise) were generated for each of the AChBP (sub)types. The AChBP/pPIC9 constructs were amplified in *E. coli* DH5 α F and isolated and purified using the plasmid Maxi Kit (Qiagen). Due to the engineered cleavage site at the N-terminus of the amino acid sequence four additional amino acids (EAEA, SEQ ID No. 16) will precede the N-terminus of the original mature protein. Prior to transfection into *Pichia pastoris* the constructs were linearised (for protocol see supplier's manual; *Pichia* Expression Kit version 3.0, Invitrogen) and subsequently purified by phenol/chloroform extraction, and ethanol precipitation. Approximately 5 μ g of each of the linearised constructs was transformed into freshly prepared electro-competent *Pichia pastoris* cells and plated onto MD plates (for protocol see supplier's manual; *Pichia* Expression Kit version 3.0, Invitrogen corporation). Electrocompetent *Pichia pastoris* cells were aquired according to the protocol provided by Invitrogen. Plates were incubated at 30°C until the appearance of *Pichia* colonies, which were subsequently analysed for the presence of the correct insert by PCR amplification (for protocol see supplier's manual; *Pichia* Expression Kit version 3.0, Invitrogen). Colonies containing an homologous recombination with the *Pichia* genome, carrying the AChBP sequence, were grown in 25 ml of BMGY for 1-2 days (30°C; rotation at 250rpm), after which the cells were centrifuged (10 min., 1500g) and the cell pellet was resuspended into 10 ml of BMMY. Growth (30°C, 250rpm) was continued for an

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additional 4 days (day 3-6), during which the expression of AChBP was induced by the addition of 100% methanol (1% of total culture volume) once every 24 hours. At day seven the culture was centrifuged (15 min.; 2000g; 4°C) and the medium was collected. The AChBP expression level of the various cultures was determined by the analyses of a fraction of the collected medium with SDS-polyacrylamide gel electrophoresis (see suppliers manual; Pichia Expression Kit version 3.0, Invitrogen). The cultures that yielded the highest level of AChBP expression were selected and stored as glycerol stocks.

Recombinant AChBP that contained a C-terminal His-tag was isolated and purified from the Pichia pastoris medium using Talon metal affinity resin (according to protocol as described within the user manual; Clontech laboratories Inc.). The protein concentration was subsequently analysed using SDS-polyacrylamide gel electrophoresis and reference marker proteins. Polyclonal antibodies have been raised successfully to the recombinant L-AChBP_T1 and B-AChBP_T1 proteins in Balb-C mice. Immune-sera were obtained without crosslinking of the proteins.

Binding characteristics of AChBP:

First the binding curve of α -Bungarotoxin to His-tagged AChBP was determined, and an affinity of 3.5 nM was calculated. Using α -Bungarotoxin in a competitive binding assay ligands of several types of ligand-gated ion channels were then tested on His-tagged AChBP, i.e., ACh, serotonin, GABA, glycine, and glutamate. Both ACh and serotonin did compete with α -Bungarotoxin binding at 4.2 mM and 269 mM, IC50s respectively. GABA, Glycine and glutamate did not compete for binding with α -Bungarotoxin. Thus, as predicted by the primary sequence and by subunit structure also the ligand-binding characteristics of AChBP resembled that of a nAChR.

In a second series of competitive binding assays the ligand binding characteristics of AChBP were studied in more detail, now using various agonists and antagonists of the AChRs. Nicotine a classical agonist of the nAChRs, is a high affinity ligand of His-tagged AChBP (IC50 98 nM). Epibatidine, a high affinity agonist of the nAChRs, also binds with high affinity to His-tagged AChBP (IC50 1.4 nM), which is even higher than the 58 pM affinity of epibatidine reported for the nAChR (Badio, Mol. Pharmacol. 45 (1994), 563-569). Other cholinergic agonists bind with a lower affinity e.g., decamethonium, carbachol, and choline respectively with IC50s of 4.1 μ M, 43 μ M, and 190 μ M. Summary of affinities indicated in Table 2.

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Table 2

| | IC ₅₀ (μM) | nHill | | IC ₅₀ (μM) | nHill |
|---------------|-----------------------|-------------|----------------|-----------------------|-------------|
| serotonin | 269 ± 67 | 0.65 ± 0.03 | α-cobratoxin | 16.2 ± 0.1 | 4.08 ± 0.30 |
| choline | 190 ± 32 | 0.91 ± 0.20 | atropine | 5.25 ± 0.49 | 1.91 ± 0.23 |
| carbachol | 43 ± 2.7 | 0.67 ± 0.05 | decamethonium | 4.1 ± 0.3 | 1.13 ± 0.09 |
| acetylcholine | 4.2 ± 1.1 | 0.72 ± 0.09 | physostigmine | 1.25 ± 0.04 | 0.66 ± 0.07 |
| nicotine | 0.098 ± 0.025 | 0.78 ± 0.05 | d-tubocurarine | 0.093 ± 0.003 | 0.83 ± 0.04 |
| epibatidine | 0.0014 ± 0.0001 | 0.66 ± 0.04 | gallamine | 0.039 ± 0.007 | 0.71 ± 0.14 |
| | | | α-bungarotoxin | 0.0026 ± 0.0006 | 0.80 ± 0.18 |

5 Competition-binding of typical antagonists of the nAChRs, e.g., tubocurarine and α-Bungarotoxin, have a high affinity for His-tagged AChBP, respectively IC₅₀s of 93 nM and 2.6 nM. The cholinergic antagonist succinylcholine has a very low affinity for His-tagged AChBP (IC₅₀ 7.9 mM). Interestingly, also muscarinic receptor antagonists bind to His-tagged AChBP with relatively high affinity, e.g., the

10 muscarinic allosteric modulator gallamine (IC₅₀ 39 nM), and the muscarinic antagonist atropine (IC₅₀ 5.3 mM). Physostigmine which is a known blocker of acetylcholinesterase and is also an antagonist of the nAChR, binds to His-tagged AChBP with an IC₅₀ of 1.3 mM.

Finally, Bipinnatin-B was tested, a synthetic form of the coral lophotoxin on AChBP

15 (Groebe and Abramson, J. Biol. Chem. 270 (1995), 281-286). Bipinnatin-B is a general blocker of nAChRs and is known to covalently bind to Tyr-190 of the α subunits (Abramson, J. Biol. Chem. 263 (1988), 18568-18573). His-tagged AChBP was incubated with the toxin, and the mass of the protein increased with 430.1 Da, corresponding well to the calculated mass of Bipinnatin-B of 431 Da, indicating that

20 the toxin also binds to Tyr-184 in His-tagged AChBP.

EXAMPLE 5: Expression and purification of recombinant AChBP for crystallization

The AChBP_T1 protein from *Lymnea stagnalis* (AChBP) was overexpressed in

25 *Pichia pastoris* GS115 strain using the AOX1 gene expression system from Invitrogen. Media and methods used for AChBP expression are also described in Invitrogen manual *Pichia* Expression Kit. For long term storage the transformants were grown overnight in YPD medium at 30°C.

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YPD or Yeast Extract Peptone Dextrose medium

1% yeast extract (Difco)

2% peptone (Difco)

2% dextrose (glucose) (Merck)

- 5 The cells were harvested and suspended in YPD medium containing 15% glycerol at final OD₆₀₀ of ~50. The cells were frozen in a dry ice/ethanol bath and stored in the freezer (Revco) at -80°C. Normally, the expression of AChBP started with plating the cells from the glycerol stock on MD plate.

MD or Minimal Dextrose Medium

- 10 1.34% YNB (yeast nitrogen base w/o amino-acids) (Difco)

4x10⁻⁵ % d-biotin (Sigma)

1% dextrose

For plates add 15g of agar (Difco)

- 15 The plate was stored in the incubator (Heraeus) for 3-4 days at 30°C. A single colony was picked from the plate and inoculated in 150 ml baffled flask (Nalgene) containing 25 ml of BMGY medium.

BMGY or Buffered Glycerol-complex Medium

1% yeast extract

2% peptone

- 20 100 mM potassium phosphate (pH 6.0) (Merck)

1.34% YNB

4x10⁻⁵ % d-biotin

1% glycerol (Merck)

- 25 The culture was placed into the shaker (New Brunswick) and left to grow overnight rotating at 250 rpm at 30°C. The following day 12.5 ml of the culture was inoculated into 225 ml of BMGY medium in a 1000 ml baffled flask. In order to increase the yield of expressed AChBP a larger number of flasks were used, usually 16. The flasks were placed in the shaker and start-cultures were rotated at 250 rpm at 30°C. After two days the start-cultures were centrifuged for 15 min at 2500 rpm (Sorvall RC3B+, rotor H-6000A) at room temperature. In order to increase the cell mass for bigger protein production, cell pellets of two start-culture flasks were pooled together and resuspended in 200 ml of BMMY medium containing 1% (w/v) casamino acids.

BMMY of Buffered Methanol-complex Medium + 1% casamino acids

1% yeast extract

- 35 2% peptone

100 mM potassium phosphate (pH 6.0)

1.34% YNB

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4x10⁻⁵ % d-biotin

0.5% methanol (Merck)

1% casamino acids (Difco)

The cultures were put back into the shaker (250 rpm, 30°C) and induced for the following 4 days. The concentration of methanol in the medium was kept constant by adding 1% (v/v) methanol to the cultures every 24 hours. After 4 days 100 ml of culture was harvested and the original volume of 200 ml was readjusted by adding fresh BMMY medium with 1% casamino acids. The remaining cultures were induced for another 4 days. The harvested cultures were centrifuged for 15 min at 4000 rpm (Sorvall RC3B+, rotor H-6000A) and the cell pellet was discarded. The supernatant was first filtered through a 0.22 µm filter (Millipore) to remove any remaining cells and it was concentrated using a Minitan system (Waters/Millipore) with 30kDa cutoff filter (Waters/Millipore). Both the filtration and concentration and were performed at 4°C. Finally, centrifugation at 16000 rpm was done (Sorvall RC5C, rotor SS-34) in order to remove any debris left after the first two steps. The final volume of concentrated sample was ~80 ml and it was dialyzed overnight against 2 x 5 l (20 mM Tris [pH 8.0], 150 mM NaCl and 0.02% NaN₃) using 15kDa cutoff dialysis membrane (Spectra/Por) at 4°C. The dialyzed protein solution (~100 ml) was loaded onto an anion-exchange column (POROS 50 HQ, Pharmacia, column volume 8 ml). After the initial wash step of ~15 column volumes using loading buffer, a salt gradient of 30 column volumes was run from 150 mM to 1000 mM NaCl. Both solutions contained also 20 mM Tris (pH 8.0) and 0.02% NaN₃. The peak of interest eluted at ~300 mM NaCl (conductivity range 16-24 mS/cm). The presence of AChBP was checked by Bio-Rad Protein Assay (Bio-Rad) and SDS-PAGE and the fractions of interested were pooled and concentrated using a Centriprep with a 30kDa cutoff membrane (Amicon). The concentrated sample (volume of 5 ml) was loaded onto a gel filtration column (Superdex 200 HR 16/60, Pharmacia, column volume 120 ml) using 20mM Tris (pH 8.0), 150 mM NaCl and 0.02% NaN₃. The protein eluted starting from 60 to 71 ml with peak at ~66 ml. The final purification step of the protein was done on an anion-exchange column (MonoQ HR10/10, Pharmacia, column volume 6 ml). The protein was loaded onto the column in the same buffer as eluted from the gel filtration column. The salt gradient used for the column was the identical to the one used for the POROS 50 HQ column. The fractions in the conductivity range 25-27.5 mS/cm were pooled together and dialyzed against buffer containing 50 mM HEPES (pH 7.0) and 0.02% NaN₃. The protein was concentrated up to ~20 mg/ml using a Centricon with a 30kDa cutoff membrane (Amicon). The total yield was about 2 mg purified

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protein per liter of expressed medium. The concentrated protein was stored at 4°C and used for crystallization experiments and biochemical characterization. N-terminal sequencing revealed the presence of EAEAYVEF residues that are part of the pIC9-encoded signal sequence, before residue 2. The experimental mass was determined to be 26544 Da (MALDI), which is ~2kDa more than calculated mass based on amino-acid sequence (24649 Da). The difference is assigned to glycosylation of AChBP at position Asn66 in the mature sequence, confirmed by deglycosylation experiments with N-glycosidase F (Boehringer).

The purification of the first harvest was done separately from the full harvest. They were pooled together prior to the last purification step (anion-exchange chromatography step on MonoQ column). All above mentioned chromatography columns were mounted on an FPLC system (Pharmacia) controlled by the UNICORN system (Pharmacia). All solutions used in the FPLC system were prepared with MilliQ UF+ water, filtered through 0.22 µm filter (Millipore) and degassed.

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EXAMPLE 6: Crystallization of the AChBP

All the crystallization experiments were done by vapor diffusion technique in a hanging drop mode using 12 well tray (Nelipak) and siliconized cover slides (Hampton Research). Trays were placed in a sandwich box (Semadeni) and stored at 19°C temperature conditioned room. The initial crystallization attempts were performed using Hampton Crystal Screen I and II (Hampton Research). Drops contained 2 µl of protein (10 mg/ml in 50 mM HEPES [pH 7.0] and 0.02% NaN₃) and 2 µl of reservoir solution. From the first screen it became clear that AChBP makes crystalline precipitate in the presence of CaCl₂ salt. A more detailed screen was made which produced crystals suitable for X-ray analysis. The AChBP crystals appeared in the following conditions: 9-11% (w/v) PEG 4000 (Hampton Research), 100 mM HEPES (pH 7.0), 50-200 mM CaCl₂ x 6H₂O and 0.02% NaN₃ or or PEG MME 550 10-18% in the same conditions, with 0.3 mM ZnAcetate as additive. Depending on the batch of the protein used and the CaCl₂ concentration three different crystal forms were found: orthorhombic, tetragonal and monoclinic. Both orthorhombic and monoclinic crystal forms are frequently twinned. Orthorhombic rod-like crystals appeared immediately upon setting up the crystallization experiments (in between first few hours) under high [CaCl₂]. The size of the crystals varied from 0.05x0.05x0.15 to 0.25x0.25x1.0 mm. The crystals diffract X-ray up to 3 Å resolution and show high degree of mosaicity (~0.5-1.2°). They have the symmetry of space group *P*2₁2₁2₁ with cell constants of a= 120.62Å, b=137.01Å, c=161.54Å with 2 pentamer molecules per asymmetric unit. Tetragonal crystals, squared in shape,

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grew at lower CaCl_2 concentration, reaching 0.2x0.3x0.35 mm in size. The maximal resolution obtained was 2.7 Å with a lower mosaicity (0.5°). They belong to space group $P4_22_12$ space group with cell dimensions of $a=b=141.66\text{Å}$, $c=120.83\text{Å}$ with one pentamer molecule per asymmetric unit. The exact crystallization condition for the tetragonal crystal which was used for refinement of the crystal structure: 11.5% (w/v) PEG 4000, 100 mM HEPES (pH 7.0), 150 mM CaCl_2 and 0.02% NaN_3 . The third crystal form, monoclinic $P2_1$, is very similar in morphology to the orthorhombic crystals with cell dimensions of $a=121.1\text{Å}$, $b=162.1\text{Å}$, $c=139.4\text{Å}$, $\beta=90.13^\circ$, containing 4 pentamers per asymmetric unit. This crystals were gave lower resolution data (~3.3Å resolution). All three crystal forms were used in the structure determination of AChBP.

The resolution limit of diffraction depended very much on the size of the crystals. And the largest crystals diffracted weakly to ~4Å resolution when exposed to a conventional rotating anode X-ray source. Therefore, the use of synchrotron radiation was critical for the structure determination. The crystals had to be cryo-protected in order to slow down the damage caused by high intensity synchrotron radiation. The cryo-protection of the AChBP crystal was done in multiple steps. The first steps included the stabilization of crystal by adding the 2 µl of mother liquor (equilibrated reservoir solution) to the drop with the crystal. After 5 minutes 3 µl of stabilizing solution was added to the drop. Normally, the stabilizing solution contained slightly higher concentrations (1-5%) of the components of the original crystallization buffer. As protectant glycerol (Merck) was added, increasing the concentration stepwise from 0% to 30% (v/v). For example, the starting solution contained 15% PEG 4000, 100 mM HEPES (pH 7.0), 150 mM CaCl_2 and 0.02% NaN_3 and the final solution contained 30% (v/v) glycerol in addition to the components just mentioned. The AChBP crystals do not tolerate drastic increase in the glycerol concentrations therefore a gentle but more time consuming approach has to be adopted. The solution around the crystal has to be stepwise exchanged (usually 5% increase of glycerol concentrations) allowing crystals to equilibrate for at least 5 minutes in each glycerol concentration. Once the crystals were equilibrated in stabilizing solution with 30% glycerol they were flash-cooled in liquid nitrogen or in the cryo-stream. In all three space groups AChBP forms a decamer structure with perfect 52 symmetry, where two pentamers contact each other through a calcium-binding site, at the 'top' of the $\alpha 1$ helix. This binding site (Asp2 and Asp5 from two monomers) is not conserved in the LGIC family. In the tetragonal space group the 2-fold of the decamer coincides with a crystallographic two-fold, which leads to

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pseudocentrosymmetric behavior of the phases at low resolution. In solution the AChBP protein acts as pentamer.

Those of skill in the art will appreciate that the aforesaid crystallization conditions can be varied. Such variations may be used alone or in combination, and include final protein (optionally in complex with a ligand) concentrations between 1 mg/ml and 30 mg/ml; all combinations of AChBP/ligand to precipitant ratios; use of citrate concentrations between 0 mM and 200 mM; DTT concentrations between 0 mM and 10 mM; and any concentration of beta-mercaptoethanol; pH ranges between 5.5 and 9.5; PEG concentrations between 5% and 25% (w/v); PEG weights between 2000 and 8000; HEPES concentrations between 5 and 500 mM; use of TRIS or other solutions instead of HEPES, and any concentration or type of detergent; any other type of precipitating agent; any other buffer; any temperature between -50 °C and 30 °C; and crystallization of AChBP or complexes thereof by batch, liquid bridge, or dialysis method using these conditions or variations thereof.

EXAMPLE 7: Structure determination

The crystal structure was determined using the multiwave anomalous dispersion (MAD) technique on a Pb derivative, but non-crystallographic symmetry (NCS) averaging was necessary to obtain interpretable electron density. Collection of native data and heavy-atom derivatives were carried out at the synchrotron beam-lines in Grenoble (ESRF/BM14 and ID14) and Hamburg (DESY/BW7A, BW7B and X11). The AChBP orthorhombic crystal was soaked in stabilizing solution containing 5 mM trimethylleadacetate (MePb) for 5 days. Data sets were collected at four different wavelengths (0.9492Å, 0.8610Å, 0.9507Å and 0.9499Å) and data were integrated and reduced using DENZO/SCALEPACK (Otwinowski and Minor (1997) Processing of X-ray diffraction data collected in oscillation mode. In *Methods in Enzymology*, Volume 276: Macromolecular Crystallography, part A. C.W. Carter and R.M. Sweet, eds. (New York: Academic Press), pp. 307-326). The program SOLVE (Terwilliger (1997) SOLVE: An automated structure solution for MAD and MIR. Edition 1.16) found 5 Pb sites which were situated on the interface between two pentamers. The Pb parameters were refined and phases calculated with SHARP (La Fortelle et al. (1997) Advances in MIR and MAD phasing: Maximum-likelihood refinement in a graphical environment, with SHARP. Proceedings of the CCP4 study weekend). Mean figure of merit (FOM) value for 4 wavelengths was 0.45. Search and optimization of 5-fold NCS operators were done using programs NCS6D and IMP (Kleywegt and Jones (1999) Software for handling macromolecular envelopes. Acta

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Crystallo., D55, 941-944). 10-fold averaging using refined NCS operators in conjunction with density modification by DM (Cowtan (1994) DM: An automated procedure for phase improvement by density modification. In Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography 31, 34-38) yielded an interpretable

5 electron density map. However, some parts of the pentamers were still not clearly defined. Therefore, a second MAD experiment was performed on the monoclinic crystals soaked in 10 mM MePb for 5 days. Data were collected for only two wavelengths, at the Pb peak (0.9479Å) and remote (0.9498Å) wavelength. The processing of the two collected data sets was done with MOSFLM (Leslie (1992)

10 Recent changes to the MOSFLM package for processing film and image plate data. In Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography, Number 26) and data were scaled with SCALA (CCP4. The CCP4 suite: programs for protein crystallography. Acta Crystallog. D50, 760-763). 10 Pb sites were identified with Solve. The Pb parameters were refined and phases calculated with SHARP in single

15 anomalous dispersion (SAD) mode using data collected at the Pb absorption peak. The NCS operators needed for 20-fold averaging were found by NCS6D and improved with IMP. 20-fold averaging and density modification by program DM further improved electron density. The initial model tracing and sequence assignment were done based on the 20-fold averaged electron density with program O (Jones et

20 al., 1991). However, parts of the molecules were not clearly defined. The electron density was further improved doing multi-crystal averaging with DMMULTI (Cowtan, 1994) using amplitudes of tetragonal, orthorhombic and native data sets and experimental phases of the orthorhombic and monoclinic MAD experiments. Initially missing parts became clearly defined and a complete model could be built. The initial

25 atomic model was refined with the program CNS (Brünger et al. (1998) Acta Crystallogr. D 54, 905-921) against a maximum-likelihood target without experimental phases contribution using tetragonal native data which extend to 2.7Å resolution. Refinement included five-fold NCS restraints, an overall anisotropic B factor and bulk solvent correction. The five-fold NCS restraints were released for the parts of the

30 pentamer that clearly do not follow the five-fold symmetry. The current model contains one pentamer of AChBP consisting of 1035 residues, 14 well-ordered solvent molecules, 5 Ca²⁺ ions, 5 Cl⁻ ions and 5 Hepes molecules, well-ordered solvent molecules and 5 HEPES molecules. The following residues are not well defined in the electron density: -8-0 (part of α -mating *S. cerevisiae* signal sequence

35 not native to AChBP EAEAYVEF; SEQ ID No. 21), 125-135, 155-165, 186-191 and 206-210.

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Electron density is detectable in the ligand-binding site of AChBP. It is presumed that a HEPES molecule could account for this extra electron density based on its chemical properties. HEPES or N-2-Hydroxyethylpiperazine-N'-2-ethanesulfonic acid contains a quaternary ammonium ion similar to ligand such as acetylcholine (ACh) and d-tubocurarine. It has been proposed that the binding of ACh would be mediated by cation- π interaction involving N^+ and π -systems of aromatic residues present in the binding site of nicotinic acetylcholine receptor. Without intending to be bound by theory it is suggested in accordance with the observation of the present invention that the observed HEPES molecule mimics ligand binding analogous to the binding of natural ligands like ACh in the ligand-binding site.

EXAMPLE 8: More detailed description of the structure determined in Example 7

As described in the previous example, the crystal structure of AChBP was solved using weak Pb MAD data in two crystal forms. The electron density map was improved substantially by cross-crystal averaging of three crystal forms with 20, 10 and 5 copies of the monomer in the asymmetric unit respectively (Table 3).

Table 1: Data collection statistics

| | Data set | λ_1 peak | λ_2 remote | λ_3 infl. | λ_1 peak | λ_2 infl. | Native |
|----|------------------------|------------------|--------------------|-------------------|------------------|-------------------|-------------|
| 20 | Space group | $P2_12_12_1$ | | | $P2_1$ | | $P4_22_12$ |
| | Resol. (Å) | 3.3/3.4-3.3 | | | 3.0/3.1-3.0 | | 2.7/2.8-2.7 |
| | λ (Å) | 0.9492 | 0.8610 | 0.9507 | 0.9479 | 0.9498 | 0.943 |
| | Compl. (%) | 99.7/99.7 | 99.6/99.6 | 99.7/99.7 | 99.9/99.9 | 99.5/99.5 | 97.8/96.5 |
| | Mosaicity (°) | 0.62 | | | 0.43 | | 0.78 |
| 25 | Redundancy | 3.7/3.8 | 3.8/3.9 | 3.7/3.8 | 3.5/2.2 | 3.2/2.0 | 6.5 |
| | R_{merge} (%) | 7.7/46.8 | 7.8/45.2 | 8.3/55.0 | 5.9/26.1 | 6.0/32.9 | 5.9/67.4 |
| | $I/\sigma I$ | 8.7/1.6 | 8.4/1.7 | 8.3/1.4 | 7.7/2.7 | 6.8/1.5 | 27.4/2.3 |

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|-------------------------|-----------|-----------|-----------|-----------|-----------|
| Phasing | ISO/ANO | ISO/ANO | ISO/ANO | ISO/ANO | ISO/ANO |
| R_{cullis} (%) | 0.74/0.89 | n.a./0.92 | 0.54/0.94 | n.a./0.74 | 0.66/0.77 |
| Phasing power | 0.57/1.2 | n.a./1.06 | 2.3/0.91 | n.a./1.1 | 0.37/1.22 |
| FOM (overall) | 0.45 | | | 0.28 | |

5

The structure was refined at 2.7 Å in space group $P4_22_12$, with one AChBP pentamer in the asymmetric unit. Thus, native data (X11) were collected and the Pb-1 data sets (BW7A) at the EMBL/DESY synchrotron in Hamburg and the Pb-2 data sets (BM14) at the ESRF, Grenoble (Table 3). Data were processed with DENZO/SCALEPACK (Otwinowski & Minor, Methods Enzymol. 276, 307-326 1997) (native) or MOSFLM (Leslie, Acta Crystallogr. D. Biol. Crystallogr. 55, 1696-1702, 1999)/SCALA (CCP4) (Pb-1, Pb-2). The Pb sites, located at the interface of two pentamers, were found for both MAD sets by SOLVE (Terwilliger, Acta Crystallogr. 55, 849-861, 1999) and heavy atom parameters were optimized with SHARP (La Fortelle et al., Methods Enzymol. 276, 472-494, 1997). NCS operators were found and refined with NCS6D and IMP (Kleywegt and Jones, SERC Daresbury Laboratory, Warrington, pp. 59-66, 1994). DM-multi (Cowtan, Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography, 31, 34-38, 1994) multi-crystal averaging used amplitudes of monoclinic, orthorhombic and native (tetragonal) data sets and experimental phases of the orthorhombic and monoclinic MAD experiments. The model was built in O (Jones et al., Acta Crystallogr. A47, 110-119, 1991) and refined with the program CNS (Brünger et al., Acta Crystallogr. D54, 905-921, 1998), against the tetragonal data to 2.7 Å resolution. Refinement included partial 5-fold NCS restraints, an overall anisotropic B factor and bulk solvent correction. The unusual double cysteine Cys187-Cys188 formed a clear disulfide bridge. Because of the limited resolution it was refined with standard parameters. The final model contains 1025 residues of AChBP pentamer, 5 HEPES molecules, 10 Ca^{2+} ions and 15 water molecules. The entire AChBP pentamer is well ordered, except for the N-terminal 7 residues (part of the signal sequence) and the last five C-terminal residues. In addition, the HEPES, the loop region 155-160 and the sugar residues attached to residue Asn66 are not well resolved in the electron density. R.m.s deviations from ideal geometry for bond distances and angles are 0.01 Å and 1.6°, respectively. The sequence alignment was calculated by CLUSTALX (Thompson et al., Nucleic. Acids. Res. 25, 4876-4882,

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1997) and the corresponding figure with Esript (Gouet et al., Bioinformatics. 15, 305-308, 1999). Figures 2-5 were done using programs MOLSCRIPT (Kraulis, P.J., J. Appl. Cryst. 24, 946-950, 1991), BOBSCRIPT (Esnouf, Acta Crystallogr. D55, 938-940, 1999) and RASTER3D (Merritt and Bacon, Methods Enzymol. 277, 505-524, 5 1997). Refinement took place with partial five-fold NCS restraints, resulting in an R-factor of 26.4% ($R_{\text{free}} = 30\%$).

The AChBP pentamer:

10 The AChBP homopentamer, when viewed along the five-fold axis, resembles a windmill toy, with petal-like monomers (Fig. 6a). When viewed perpendicular to the five-fold axis it has a disc-like appearance (Fig. 6b). The overall proportions of the pentamer are $\sim 80 \times 80 \times 62$ Å, and the diameter of the central hole is ~ 18 Å. These dimensions are in good agreement with the *Torpedo* nAChR N-terminal domain EM data (Miyazawa et al., J. Mol. Biol. 288, 765-786, 1999). The only subunit contacts in 15 the AChBP pentamer are dimer interfaces, of which each monomer has two, one called the plus side and one called the minus side. We refer to the A (plus)-B (minus) interface, as example for the five equivalent interfaces AB, BC, CD, DE and EA (Fig 6).

The AChBP monomer:

20 Each AChBP monomer is a single domain protein, asymmetric in shape, with a size of $\sim 50 \times 21 \times 27$ Å (Fig. 12a). It consists of an N-terminal β -helix, two short 3_{10} helices and a core of 10 β -strands forming a β -sandwich. The order of β -strands conforms to a modified immunoglobulin (Ig) topology (Fig. 12b) with an extra β -hairpin (f'-f'') and 25 an extra strand (b') (Bork et al., J. Mol. Biol. 242, 309-320, 1994). These additional strands introduce two so-called "Greek key" folding motifs. The Ig-based structure prediction (Le Novère et al., 1999; Corringer et al., Biophys. J. 76, 2329-2345, 1999) agrees well with the AChBP structure, although location of the binding site was missed due to the presence of extra β -strands (Fig. 12b). Compared to the classical 30 Ig-fold, the AChBP β -strands are considerably twisted, with the β -sheets rotated against each other, resulting in two separate hydrophobic cores. Thus the three-dimensional fold does not resemble other Ig-like proteins and comparison to the protein database (Holm and Sander, Nucleic. Acids. Res. 25, 231-234, 1997) did not result in a significant match to any known structure.

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Positioning of functional regions:

Couple of regions that are important to receptor function can be localized in the AChBP structure. In muscle type nAChRs the main immunogenic region (MIR), comprising residues α_1 67- α_1 76, acts as an epitope in the autoimmune disease myasthenia gravis (Tzartos et al., Mol. Neurobiol. 5, 1-29, 1991). Although the MIR-related region in AChBP (residues 65-72) shows no sequence homology to the α_1 -subunit, its location in loop L3 at the top of the pentamer in a highly accessible position agrees well with the expected accessibility for this region. It also fits with EM studies that located the MIR at the distal end of the receptor relative to the membrane (Beroukhim and Unwin, Neuron 15, 323-331, 1995).

On each AChBP monomer, a large cavity that is accessible from the central pore of the pentameric ring can be seen. The cavity is framed at the entrance by β -strands (β_3 , β_4 , β_5 and β_5') (Fig 12a) and is uncharged, mainly hydrophobic, in character. This region probably corresponds to the tunnel framed by twisted β -strands that was observed in the α_1 -subunit of *Torpedo* receptor at 4.6 Å resolution (Miyazawa et al., J. Mol. Biol. 288, 765-786, 1999). However, this cavity is not in contact with another large pocket observed at each interface between subunits. These latter pockets are lined by residues shown to be involved in ligand binding in nAChR (Arias, Neurochem. Int. 36, 595-645, 2000; Corringer et al., Annu. Rev. Pharmacol. Toxicol. 40, 431-458, 2000). They are buried from the solvent, and located close to the outside of the pentameric ring. When viewed perpendicular to the five-fold axis they are roughly equatorially positioned, ~30 Å away from the C-termini (Fig. 6b), conforming to the expected location of the *Torpedo* receptor ligand-binding site, as determined by labeling (Fernando Valenzuela et al., Biophys. J. 66, 674-682, 1994) and EM studies (Unwin, J. Mol. Biol. 229, 1101-1124, 1993).

The ligand-binding site:

Each ligand-binding site is found in a cleft formed by a series of loops from the principal face of one subunit and a series of β -strands from the complementary face of an adjacent subunit. It is a large cavity buried by a series of loops from the principal side and by a β -strands from the complementary side (Fig. 13). The principal side on the plus side of the AB interface consists of residues coming from 'loop A' (TyrA89), 'loop B' (TrpA143, A145) and 'loop C' (TyrA185, the double cysteine A187-A188, and TyrA192) (Fig 13c). The complementary part of this binding

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site is contributed by monomer B and made of 'loop D' (TrpB53, GlnB55), 'loop E' (ArgB104, ValB106, LeuB112 and MetB114) and 'loop F' (TyrB164) (Fig 13d). In this pocket four of the aromatic residues form the bottom half of the cavity (TyrA89, TyrA185, TyrB164 and TrpB53). The pocket walls are formed by the TyrA192, TrpA143, main chain of A145 Met B114, the side-chain of GlnB55 and the double cysteine (CysA187-CysA188). The hydrophobic parts of ArgB104, ValB106 and LeuB112 form the top of the pocket (Fig 13a).

All residues in the pocket had been successfully identified by photoaffinity labeling and mutagenesis studies (Arias, Neurochem. Int. 36, 595-645, 2000; Corringer et al., Annu. Rev. Pharmacol. Toxicol. 40, 2000). Although the side chain of HisA145 is pointing away from the cavity, its main chain is involved. One residue identified by labeling studies, TrpA82 (α_1 Trp86) (Galzi et al., J. Biol. Chem. 265, 10430-10437, 1990; Dennis et al., Biochemistry 27, 2346-2357, 1988) is involved in hydrophobic core formation and located far from the pocket, thus not participating in ligand binding. Otherwise, the AChBP ligand-binding site confirms the available biochemical and mutational data on nAChR completely.

The structure, however, shows for the first time how these residues are positioned with respect to each other and therefore provide a valuable tool for drug design as described in the above description of the present invention.

All observed residues are conserved between known nicotinic ligand-binding subunits except the 'loop F' TyrB164 residue. The 'loop F' region has an unusual conformation, but since it is relatively weakly resolved, its precise analysis is difficult. The 'loop F' region is stabilized in the structure by a calcium binding site formed by AspB161, AspB175 and the main chain of B176. This Ca^{2+} ion is structurally important for TyrB164 orientation and could therefore be important for proper ligand binding. The present findings are supported by labeling studies on muscle/*Torpedo* subunits showing that residues homologous to AspB161, γ Asp174/ δ Asp180 play a role in ligand binding (Czajkowski et al., Proc. Natl. Acad. Sci. U.S.A. 90, 6285-6289, 1993; Czajkowski and Karlin, J. Biol. Chem. 270, 3160-3164, 1995; Martin et al., J. Biol. Chem. 271, 13497-13503, 1996). Additionally, calcium binding sites that enhance the response to agonist binding have been identified in the homologous region (residue range 161-172) of neuronal α_7 receptor (Galzi et al., EMBO J. 15, 5824-5832, 1996). The 'loop F' region has low sequence conservation in the nicotinic family (Fig. 11) and in other superfamily members it may well have a different conformation, even to the extent of forming a β -strand that connects the two sheets

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into a β -barrel. Such changes could well lead to variations in affinity, *e.g.* by changing the size of the ligand-binding site or its access route.

5 The most likely access routes to the ligand binding sites are from above or below the double-cysteine-containing 'loop C' (Fig. 13a). This region buries the pocket from the solvent and therefore prevents access from the outside. Access from the central pore has been suggested in the literature (Miyazawa, J. Mol. Biol. 288, 765-786, 1999), but this would require major structural rearrangements at the interface, which makes it less likely.

10

Ligand binding:

Surprisingly, features of bulky electron density were found that stacked onto Trp143 in each ligand-binding site in the experimental cross-crystal averaged electron density (Fig 13b). Upon consideration we have assigned this to a HEPES (N-2-
15 Hydroxyethylpiperazine-N'-2-ethanesulfonic acid) buffer molecule, that contains a positively charged quaternary ammonium group and therefore has some similarity to known nicotinic receptor ligands. Its EC50 is 100 mM, indicating that its binding under crystallization conditions (100-150 mM) is possible. Although HEPES molecule does not make any specific contacts with the protein, it stacks with its quaternary
20 ammonium onto Trp143, making cation- π interactions as expected for nicotinic agonists (Dougherty, Science 271, 163-168, 1996) (Fig. 13b). However, due to limited resolution of the present data and probable low occupancy, the precise orientation of the HEPES molecule should be taken with some degree of reservation.

25 It has been suggested (Changeux and Edelstein, Neuron 21, 959-980, 1998) that the ligand-binding site of nAChRs could be similar to that of acetylcholinesterase (AChE). Although the size of the binding site is roughly similar in AChBP and AChE, the observed arrangement of aromatic residues is quite different. However, the stacking of the quaternary ammonium of HEPES, as far as it has been refined in the current
30 AChBP structure, is similar to that of the quaternary ammonium of the decamezonium in AChE on the Trp84 residue (Harel et al., Proc. Natl. Acad. Sci. U.S.A. 90, 9031-9035, 1993).

Subunit arrangement:

35 From the location of the ligand-binding site conclusions can be drawn about the relative arrangement of subunits in the *Torpedo* and muscle receptors. It has been suggested that the $\alpha_1\gamma$ and $\alpha_1\delta$ interfaces occur in a clockwise $\alpha_1\gamma\alpha_1\delta\beta_1$ arrangement

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when looking towards the membrane (Machold et al., Eur. J. Biochem. 234, 427-430, 1995). Such a clockwise arrangement disagrees with the structure determined in accordance with the present invention, because the relative arrangement of the principal binding site and its complementary partner is anticlockwise when looking
5 towards the 'bottom' (membrane) side of the pentamer (Fig. 6).

Pentamer interface:

The subunit interface consists on the plus side entirely of loop regions (L1, L2, L4, L5, L7, L8 and L10), whereas the minus side mostly presents secondary structure
10 elements to the interface ($\alpha 1$, $\beta 1$, $\beta 2$, $\beta 3$, $\beta 5$, $\beta 6$ and L9) (Fig. 14). Several residues are important for both ligand-binding and pentamer formation. The interface buries a considerably surface area (2700 \AA^2), with a mainly uncharged character including only a single bifurcated salt bridge (GluA149-ArgB3 and ArgB104). Most intriguing
15 about the interface residues is the lack of conservation of these particular residues in the entire superfamily, not only with AChBP, but also amongst each other (Fig. 11). These changes involve major changes in character, including changes from hydrophobic to charged. Even when a residue is conserved in any particular subunit, its expected counterpart is missing (either in the same subunit, as in the α_7
20 homopentamers, or in contacts such as muscle $\alpha_1\delta$ or $\alpha_1\gamma$ or neuronal $\alpha_4\beta_2$) with the sole exception of the ligand-binding site. The high level of structural conservation however, determines involvement of the same topological regions in these contacts in all family members (Fig 14b). This indicates that shape complementarity must play a major role in determining the conservation of the pentamer structure. It also
25 indicates that different combinations of subunits will have different interfaces, creating variations in the precise allosteric contacts and movements in the various subclasses of these ion channels.

Ligand-gated ion channels:

The lack of conservation of the interface residues seems a general feature in the
30 superfamily of LGICs, as the residues that form the interface are among the least conserved regions of the domains (Fig. 11). Apparently pentamer formation does not impose very stringent evolutionary requirements in this case. However, there is clear sequence conservation within the superfamily (Fig. 11) and it is interesting to analyze
35 this in the light of the structure.

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In the AChBP monomer structure the conserved hydrophobic residues can be grouped into three clusters (Fig. 15). In AChBP, as in other proteins with Ig-like fold, the packing of the β -sheets is promoted mainly by hydrophobic and to a lesser extent by electrostatic interactions. The first cluster is involved in packing of the N-terminal helix $\alpha 1$ against the main framework of the monomer and it involves residues 6, 10, 63, 65, 71, 81, 105 and 111. The second cluster, comprising residues 20, 27, 29, 31, 58, 82, 84, 86, 140, 150, 152 and 195, is situated in the upper half of the β -core region. The third cluster, including residues 33, 35, 38, 41, 48, 52, 125, 138, 171, 173, 199 and 201, is located at the lower end of the structure (Fig 15). The only non-hydrophobic residues that are highly conserved in the superfamily are Asp60, Asp85, Asn90 and Gly109. Asp60 and Gly109 are involved stabilizing the turns of a Greek key motif connecting strands $\beta 3$, $\beta 5$, $\beta 6$ and $\beta 2$, where Asp60 stabilizes the N-terminus of a small 3_{10} helix and Gly109 enables tight turn formation. Conserved residues Asp85 and Asn90 are involved in packing of the β -sheets. Asp85 forms hydrogen bonds to the highly conserved Ser142 and Thr144 and residue Asn90 brings together the main-chain oxygens of Ser122 and Arg137, enabling disulfide bond formation of the nearby absolutely conserved disulfide bond (123-136). This disulphide bond is topologically equivalent to so-called 'tyrosine cornerstone' (Hemmingsen et al., Protein Sci. 3, 1927-1937, 1994), which links the two β -sheets together in Ig-like proteins. This explains why in the *Torpedo* receptor the Cys128-Cys142 bond is important for both preservation of subunit conformational stability (Mishina et al., Nature 313, 364-369, 1985) and complete nAChR assembly (Green & Wanamaker, J. Neurosci. 18, 5555-5564, 1998). Since the observed overall structural conservation is high, it is clear that all LGIC N-terminal domains will have the same three-dimensional structure.

In contrast to the above residues, the Cys-loop is a highly conserved hydrophobic region in the LGIC family but presents a totally different character in AChBP (Fig. 11).

In AChBP, this loop is hydrophilic and is found at the bottom (membrane) side of the protein, at the dimer interface. This location and its hydrophobicity in the LGIC family implies that this loop could interact with the membrane or with the transmembrane region of the receptors, functions that are absent in AChBP.

Since all ligand gated ion channels have intrinsically the same function, opening of a membrane pore, it is likely that the conserved regions of the protein determine this function. That also indicates that it is unlikely that the interface of the pentamer has a major role in opening the channel. It is possible that the conserved Cys-loop is

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directly involved in transmitting this kind of information to the membrane part of the LGICs. Another option is that large structural changes in the β -sheet regions play a role in opening the channel. Indeed, the movement observed at 9 Å for *Torpedo* nAChR upon agonist binding (Unwin, Nature 373, 37-43, 1995), fits well with such a suggestion. In accordance with the present invention a twisted β -sandwich would be observed, with two distinct hydrophobic cores and it is entirely possible that these cores move with respect to each other upon ligand binding. The effect of such movements will then be modulated by the varying subunit interfaces in the different subtypes of the receptor, allowing intricate specificity in the neuronal signal transmission.

EXAMPLE 9: Ligand-binding crystallization studies

AChBP was cocrystallized in complex with α -bungarotoxin (α BTX, Sigma). Prior to the crystallization experiments the stability of the complex has been investigated. Using gel-filtration chromatography (Superdex 200 HR 10/30, Pharmacia, column volume 24 ml) it has been found that it is possible to purify stable complex between AChBP and α BTX. The gel-filtration run was performed using 20 mM Tris (pH 8.0), 150 mM NaCl and 0.02% NaN_3 . The stability of the complex was also confirmed with native PAGE. The crystallization experiments were done based on the same set of conditions found to work for AChBP alone; see Example 6. A small screen was set up with different precipitant concentrations and various AChBP: α BTX concentrations. Tiny crystals appeared in the conditions containing 10-12% PEG 4000, 100 mM HEPES (pH 7.0), 20-80 mM CaCl_2 and 0.02% NaN_3 . The best looking crystals grew under above mentioned conditions when AChBP: (BTX were mixed in 1:10 molar ratio. In order to check if complex indeed crystallized, crystals were thoroughly washed, dissolved in denaturing buffer and checked on SDS-PAGE that clearly showed that they contained both proteins.

In addition, a number of small ligands were bound to AChBP in soaking experiments. These include: B-bippinatin (a synthetic analog of Iophotoxin), acetylcholine (ACh, Sigma), d-tubocurarine chloride (Sigma), carbamylcholine chloride (CCh, Sigma), galanthamine hydrobromide (Sigma), epibatidine (Sigma) and nicotine (Sigma). The soaking solutions were made of stabilizing solutions (see Example 6) and together with dissolved ligands (ligands were normally dissolved in 20 mM HEPES [pH 7.0]). The ligand concentrations used were dependent on its binding constants, as determined by ligand-binding studies. The soaking times were different depending on the ligand used. After the soaking step the crystals were flash-cooled in liquid nitrogen.

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EXAMPLE 10: Generating human alpha7 nAChR / AChBP chimeras

The chimeric proteins of nAChR subunits and AChBP can be used as tools in the development of novel, nAChR subtype specific ligands. As a first step in developing these tools chimeric proteins have been designed and constructed in which part(s) of the human alpha7 nAChR were grafted into AChBP. Previous studies on the molecular determinants of ligand-binding by the alpha7 nAChR have identified three amino acid domains that compose the primary part of the ligand-binding site, further referred to as "loops A, B, and C". Within each of the three loops amino acid residues are present that are thought to directly interact with the ligand. Based on sequence conservation of the nAChR and AChBP the three possible ligand-binding loops of AChBP have been pin-pointed in accordance with the present invention as follows: loop A, Trp-101 -> Tyr-108; loop B, Trp-162 -> His-164; loop C, Tyr-204 -> Tyr-211. The chimeric proteins that were constructed replace either one (A, B or C) or multiple (A&B, A&C, B&C and A&B&C) of the ligand-binding loops of AChBP with the corresponding human alpha7 nAChR sequence.

The loop-A domain of AChBP was replaced by the corresponding domain of the human alpha7 nAChR using a two-step polymerase chain reaction (PCR). In the first step two separate PCR amplifications (35 cycles: 94 °C; 30 sec., 58 °C; 30 sec and 72 °C; 60 sec.) yielded two halves of the chimera construct. AChBP cDNA (wild type) was used as template, and outer primers located either just before the start codon (gcgctcgagaaaagagaggctgaagcttggaccgggcagacatctt; SEQ ID No. 17) or just before the stop codon (cgcgattcaagaatttcggagcgtccctt; SEQ ID No. 18) were each used in combination with two internal primers gtggaaaccagacattctctctacaacgccatctcgaaacc (SEQ ID No. 19) and gaggagaatgtctgttccacaaagagcttattggcac (SEQ ID No. 20), respectively. The internal primers contained a 5'-tag-sequence that encoded for the introduced alpha7 nAChR domain. As such the two generated chimeric PCR products share a common tag containing a part of the alpha7 nAChR subunit. In the second step, the two PCR products from the first round were pooled and, in the absence of primers, went through 5 rounds of PCR amplification (94 °C; 30 sec., 54 °C; 3 min. and 72 °C; 90 sec.). This allowed the two halves of the chimera to anneal to each other at the common alpha7 nAChR tag. The subsequent addition of the two outer primers and another 35 cycles of 25 PCR amplification (94 °C; 30 sec., 58 °C; 30 sec. and 72 °C; 90 sec.) yielded the final chimera construct. All PCR amplifications were hot-started and performed using PFU DNA-polymerase (Invitrogen). The loop-A AChBP/alpha7 chimera was cloned, using XhoI/EcoRI restriction sites in the outer primers, into the His-tag containing yeast expression

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vector pPIC9 (Invitrogen). Validation of the construct was achieved by DNA sequencing. Expression of the chimera construct was achieved according to the *Pichia pastoris* protein expression protocol of Invitrogen.

- 5 As described in the examples and the description, the present invention provides water-soluble ligand-binding proteins derived from molluscs and analogs of ligand-gated ion channels, crystals thereof and their use for screening ligands of ligand-gated ion channels. In particular, ligand-binding proteins have been identified that are capable of forming multimers and are amenable to crystallization. The crystall
- 10 structure of one these proteins, an acetylcholine binding protein (AChBP) is provided, which can be used to generate 3D models of the extracellular ligand-binding domain of ligand-gated ion channels and thus for screening of drugs that act on these ion channels. Furthermore, chimeric proteins are provided that are capable of binding a ligand of a ligand-gated receptor, and comprising at least the amino acids of the
- 15 AChBP determining solubility of the AChBP, in the same positions as in the AChBP, and furthermore comprising amino acids determining binding to said ligand.

It will be clear that the invention may be practiced otherwise than as particularly described in the foregoing description and examples. Numerous modifications and variations of the present invention are possible in light of the above teachings and,

20 therefore, are within the scope of the appended claims.

The entire disclosure of each document cited (including patents, patent applications, journal articles, abstracts, laboratory manuals, books, or other disclosures) in the Background of the Invention, Description, and Examples is hereby incorporated herein by reference. Moreover, the sequence listing is herein incorporated by

25 reference.

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Table 1

| | | | | | | | | | | |
|-----------------------------------|--------|----------|----------|----------|-------|--------|----------|--------|------|---------|
| REMARK Written by O version 7.0.1 | | | | | | | | | | |
| | CRYST1 | 141.660 | 141.660 | 120.870 | 90.00 | 90.00 | 90.00 | | | |
| 5 | ORIGX1 | 1.000000 | 0.000000 | 0.000000 | | | 0.000000 | | | |
| | ORIGX2 | 0.000000 | 1.000000 | 0.000000 | | | 0.000000 | | | |
| | ORIGX3 | 0.000000 | 0.000000 | 1.000000 | | | 0.000000 | | | |
| | SCALE1 | 0.007059 | 0.000000 | 0.000000 | | | 0.000000 | | | |
| | SCALE2 | 0.000000 | 0.007059 | 0.000000 | | | 0.000000 | | | |
| 10 | SCALE3 | 0.000000 | 0.000000 | 0.008273 | | | 0.000000 | | | |
| | ATOM | 1 | CB | PHE A | 1 | 65.468 | 25.127 | 1.161 | 1.00 | 73.24 6 |
| | ATOM | 2 | CG | PHE A | 1 | 64.224 | 24.803 | 0.370 | 1.00 | 76.49 6 |
| | ATOM | 3 | CD1 | PHE A | 1 | 63.433 | 25.819 | -0.178 | 1.00 | 77.52 6 |
| | ATOM | 4 | CD2 | PHE A | 1 | 63.798 | 23.471 | 0.244 | 1.00 | 78.15 6 |
| 15 | ATOM | 5 | CE1 | PHE A | 1 | 62.224 | 25.522 | -0.840 | 1.00 | 79.11 6 |
| | ATOM | 6 | CE2 | PHE A | 1 | 62.590 | 23.148 | -0.412 | 1.00 | 79.82 6 |
| | ATOM | 7 | CZ | PHE A | 1 | 61.797 | 24.179 | -0.958 | 1.00 | 79.89 6 |
| | ATOM | 8 | C | PHE A | 1 | 66.638 | 27.146 | 1.923 | 1.00 | 69.89 6 |
| | ATOM | 9 | O | PHE A | 1 | 67.034 | 26.519 | 2.903 | 1.00 | 70.26 8 |
| 20 | ATOM | 10 | N | PHE A | 1 | 67.407 | 25.990 | -0.118 | 1.00 | 71.31 7 |
| | ATOM | 11 | CA | PHE A | 1 | 66.214 | 26.375 | 0.689 | 1.00 | 70.93 6 |
| | ATOM | 12 | N | ASP A | 2 | 66.562 | 28.478 | 1.909 | 1.00 | 68.78 7 |
| | ATOM | 13 | CA | ASP A | 2 | 66.958 | 29.233 | 3.105 | 1.00 | 68.57 6 |
| | ATOM | 14 | CB | ASP A | 2 | 67.577 | 30.615 | 2.739 | 1.00 | 69.98 6 |
| 25 | ATOM | 15 | CG | ASP A | 2 | 66.639 | 31.523 | 1.914 | 1.00 | 73.55 6 |
| | ATOM | 16 | OD1 | ASP A | 2 | 67.059 | 32.068 | 0.844 | 1.00 | 73.75 8 |
| | ATOM | 17 | OD2 | ASP A | 2 | 65.485 | 31.714 | 2.349 | 1.00 | 75.27 8 |
| | ATOM | 18 | C | ASP A | 2 | 65.794 | 29.374 | 4.102 | 1.00 | 67.66 6 |
| | ATOM | 19 | O | ASP A | 2 | 64.622 | 29.273 | 3.719 | 1.00 | 68.25 8 |
| 30 | ATOM | 20 | N | ARG A | 3 | 66.126 | 29.560 | 5.386 | 1.00 | 65.60 7 |
| | ATOM | 21 | CA | ARG A | 3 | 65.131 | 29.703 | 6.453 | 1.00 | 60.77 6 |
| | ATOM | 22 | CB | ARG A | 3 | 65.765 | 30.222 | 7.737 | 1.00 | 60.30 6 |
| | ATOM | 23 | CG | ARG A | 3 | 66.393 | 29.174 | 8.604 | 1.00 | 59.51 6 |
| | ATOM | 24 | CD | ARG A | 3 | 66.375 | 29.629 | 10.048 | 1.00 | 61.41 6 |
| 35 | ATOM | 25 | NE | ARG A | 3 | 66.440 | 28.471 | 10.927 | 1.00 | 61.03 7 |
| | ATOM | 26 | CZ | ARG A | 3 | 67.550 | 27.787 | 11.159 | 1.00 | 62.03 6 |
| | ATOM | 27 | NH1 | ARG A | 3 | 68.692 | 28.169 | 10.586 | 1.00 | 60.01 7 |
| | ATOM | 28 | NH2 | ARG A | 3 | 67.509 | 26.694 | 11.918 | 1.00 | 62.76 7 |
| | ATOM | 29 | C | ARG A | 3 | 64.034 | 30.659 | 6.055 | 1.00 | 59.92 6 |
| 40 | ATOM | 30 | O | ARG A | 3 | 62.883 | 30.487 | 6.454 | 1.00 | 59.64 8 |
| | ATOM | 31 | N | ALA A | 4 | 64.395 | 31.685 | 5.291 | 1.00 | 57.25 7 |
| | ATOM | 32 | CA | ALA A | 4 | 63.404 | 32.641 | 4.836 | 1.00 | 55.16 6 |
| | ATOM | 33 | CB | ALA A | 4 | 64.065 | 33.782 | 4.088 | 1.00 | 53.78 6 |
| | ATOM | 34 | C | ALA A | 4 | 62.421 | 31.917 | 3.927 | 1.00 | 54.69 6 |
| 45 | ATOM | 35 | O | ALA A | 4 | 61.213 | 32.062 | 4.074 | 1.00 | 55.60 8 |
| | ATOM | 36 | N | ASP A | 5 | 62.942 | 31.127 | 2.995 | 1.00 | 54.79 7 |
| | ATOM | 37 | CA | ASP A | 5 | 62.097 | 30.392 | 2.060 | 1.00 | 55.84 6 |
| | ATOM | 38 | CB | ASP A | 5 | 62.937 | 29.580 | 1.058 | 1.00 | 56.83 6 |
| | ATOM | 39 | CG | ASP A | 5 | 63.918 | 30.437 | 0.278 | 1.00 | 59.97 6 |
| 50 | ATOM | 40 | OD1 | ASP A | 5 | 63.519 | 31.519 | -0.213 | 1.00 | 61.60 8 |
| | ATOM | 41 | OD2 | ASP A | 5 | 65.095 | 30.025 | 0.148 | 1.00 | 62.19 8 |
| | ATOM | 42 | C | ASP A | 5 | 61.176 | 29.443 | 2.815 | 1.00 | 55.90 6 |
| | ATOM | 43 | O | ASP A | 5 | 60.011 | 29.268 | 2.445 | 1.00 | 53.57 8 |
| | ATOM | 44 | N | ILE A | 6 | 61.695 | 28.832 | 3.877 | 1.00 | 55.26 7 |
| 55 | ATOM | 45 | CA | ILE A | 6 | 60.890 | 27.889 | 4.650 | 1.00 | 55.12 6 |
| | ATOM | 46 | CB | ILE A | 6 | 61.743 | 27.107 | 5.657 | 1.00 | 55.82 6 |
| | ATOM | 47 | CG2 | ILE A | 6 | 60.878 | 26.056 | 6.354 | 1.00 | 53.18 6 |
| | ATOM | 48 | CG1 | ILE A | 6 | 62.924 | 26.455 | 4.933 | 1.00 | 56.24 6 |
| | ATOM | 49 | CD1 | ILE A | 6 | 63.802 | 25.568 | 5.816 | 1.00 | 59.65 6 |
| 60 | ATOM | 50 | C | ILE A | 6 | 59.742 | 28.561 | 5.396 | 1.00 | 54.71 6 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 51 | O | ILE | A | 6 | 58.589 | 28.159 | 5.256 | 1.00 | 55.75 | 8 |
| | ATOM | 52 | N | LEU | A | 7 | 60.058 | 29.583 | 6.182 | 1.00 | 52.58 | 7 |
| | ATOM | 53 | CA | LEU | A | 7 | 59.041 | 30.299 | 6.929 | 1.00 | 51.88 | 6 |
| | ATOM | 54 | CB | LEU | A | 7 | 59.697 | 31.387 | 7.784 | 1.00 | 51.65 | 6 |
| 5 | ATOM | 55 | CG | LEU | A | 7 | 60.589 | 30.828 | 8.895 | 1.00 | 51.59 | 6 |
| | ATOM | 56 | CD1 | LEU | A | 7 | 61.484 | 31.902 | 9.480 | 1.00 | 51.45 | 6 |
| | ATOM | 57 | CD2 | LEU | A | 7 | 59.700 | 30.225 | 9.953 | 1.00 | 51.32 | 6 |
| | ATOM | 58 | C | LEU | A | 7 | 58.048 | 30.915 | 5.961 | 1.00 | 51.46 | 6 |
| | ATOM | 59 | O | LEU | A | 7 | 56.846 | 30.921 | 6.204 | 1.00 | 51.87 | 8 |
| 10 | ATOM | 60 | N | TYR | A | 8 | 58.561 | 31.417 | 4.848 | 1.00 | 51.83 | 7 |
| | ATOM | 61 | CA | TYR | A | 8 | 57.727 | 32.041 | 3.832 | 1.00 | 53.61 | 6 |
| | ATOM | 62 | CB | TYR | A | 8 | 58.601 | 32.520 | 2.672 | 1.00 | 55.43 | 6 |
| | ATOM | 63 | CG | TYR | A | 8 | 57.806 | 33.119 | 1.543 | 1.00 | 57.65 | 6 |
| | ATOM | 64 | CD1 | TYR | A | 8 | 57.217 | 34.379 | 1.668 | 1.00 | 58.24 | 6 |
| 15 | ATOM | 65 | CE1 | TYR | A | 8 | 56.439 | 34.914 | 0.644 | 1.00 | 58.94 | 6 |
| | ATOM | 66 | CD2 | TYR | A | 8 | 57.601 | 32.407 | 0.366 | 1.00 | 58.93 | 6 |
| | ATOM | 67 | CE2 | TYR | A | 8 | 56.825 | 32.930 | -0.665 | 1.00 | 60.13 | 6 |
| | ATOM | 68 | CZ | TYR | A | 8 | 56.244 | 34.183 | -0.518 | 1.00 | 60.03 | 6 |
| | ATOM | 69 | OH | TYR | A | 8 | 55.453 | 34.699 | -1.527 | 1.00 | 63.97 | 8 |
| 20 | ATOM | 70 | C | TYR | A | 8 | 56.636 | 31.114 | 3.296 | 1.00 | 52.67 | 6 |
| | ATOM | 71 | O | TYR | A | 8 | 55.483 | 31.511 | 3.143 | 1.00 | 52.13 | 8 |
| | ATOM | 72 | N | ASN | A | 9 | 57.009 | 29.880 | 2.997 | 1.00 | 53.39 | 7 |
| | ATOM | 73 | CA | ASN | A | 9 | 56.051 | 28.918 | 2.488 | 1.00 | 53.87 | 6 |
| | ATOM | 74 | CB | ASN | A | 9 | 56.750 | 27.613 | 2.096 | 1.00 | 58.21 | 6 |
| 25 | ATOM | 75 | CG | ASN | A | 9 | 57.646 | 27.772 | 0.860 | 1.00 | 62.45 | 6 |
| | ATOM | 76 | OD1 | ASN | A | 9 | 57.647 | 28.824 | 0.209 | 1.00 | 64.72 | 8 |
| | ATOM | 77 | ND2 | ASN | A | 9 | 58.405 | 26.724 | 0.530 | 1.00 | 62.99 | 7 |
| | ATOM | 78 | C | ASN | A | 9 | 54.987 | 28.638 | 3.526 | 1.00 | 53.31 | 6 |
| | ATOM | 79 | O | ASN | A | 9 | 53.794 | 28.725 | 3.239 | 1.00 | 52.02 | 8 |
| 30 | ATOM | 80 | N | ILE | A | 10 | 55.420 | 28.300 | 4.736 | 1.00 | 53.77 | 7 |
| | ATOM | 81 | CA | ILE | A | 10 | 54.489 | 28.018 | 5.829 | 1.00 | 55.18 | 6 |
| | ATOM | 82 | CB | ILE | A | 10 | 55.229 | 27.788 | 7.150 | 1.00 | 53.51 | 6 |
| | ATOM | 83 | CG2 | ILE | A | 10 | 54.220 | 27.639 | 8.272 | 1.00 | 53.99 | 6 |
| | ATOM | 84 | CG1 | ILE | A | 10 | 56.109 | 26.541 | 7.044 | 1.00 | 50.48 | 6 |
| 35 | ATOM | 85 | CD1 | ILE | A | 10 | 57.043 | 26.346 | 8.202 | 1.00 | 47.68 | 6 |
| | ATOM | 86 | C | ILE | A | 10 | 53.523 | 29.183 | 6.032 | 1.00 | 57.42 | 6 |
| | ATOM | 87 | O | ILE | A | 10 | 52.319 | 28.997 | 6.221 | 1.00 | 57.74 | 8 |
| | ATOM | 88 | N | ARG | A | 11 | 54.070 | 30.390 | 5.997 | 1.00 | 58.29 | 7 |
| | ATOM | 89 | CA | ARG | A | 11 | 53.283 | 31.600 | 6.156 | 1.00 | 60.48 | 6 |
| 40 | ATOM | 90 | CB | ARG | A | 11 | 54.199 | 32.810 | 6.042 | 1.00 | 64.72 | 6 |
| | ATOM | 91 | CG | ARG | A | 11 | 53.513 | 34.134 | 6.270 | 1.00 | 70.99 | 6 |
| | ATOM | 92 | CD | ARG | A | 11 | 53.241 | 34.337 | 7.757 | 1.00 | 79.75 | 6 |
| | ATOM | 93 | NE | ARG | A | 11 | 53.059 | 35.751 | 8.105 | 1.00 | 86.33 | 7 |
| | ATOM | 94 | CZ | ARG | A | 11 | 53.848 | 36.733 | 7.665 | 1.00 | 89.85 | 6 |
| 45 | ATOM | 95 | NH1 | ARG | A | 11 | 54.871 | 36.451 | 6.845 | 1.00 | 92.68 | 7 |
| | ATOM | 96 | NH2 | ARG | A | 11 | 53.636 | 37.992 | 8.056 | 1.00 | 90.02 | 7 |
| | ATOM | 97 | C | ARG | A | 11 | 52.204 | 31.701 | 5.082 | 1.00 | 59.54 | 6 |
| | ATOM | 98 | O | ARG | A | 11 | 51.038 | 31.954 | 5.363 | 1.00 | 59.64 | 8 |
| | ATOM | 99 | N | GLN | A | 12 | 52.614 | 31.489 | 3.841 | 1.00 | 59.22 | 7 |
| 50 | ATOM | 100 | CA | GLN | A | 12 | 51.718 | 31.595 | 2.705 | 1.00 | 58.15 | 6 |
| | ATOM | 101 | CB | GLN | A | 12 | 52.542 | 31.776 | 1.441 | 1.00 | 59.05 | 6 |
| | ATOM | 102 | CG | GLN | A | 12 | 52.118 | 32.961 | 0.629 | 1.00 | 60.64 | 6 |
| | ATOM | 103 | CD | GLN | A | 12 | 52.674 | 34.226 | 1.192 | 1.00 | 61.53 | 6 |
| | ATOM | 104 | OE1 | GLN | A | 12 | 53.879 | 34.345 | 1.360 | 1.00 | 65.50 | 8 |
| 55 | ATOM | 105 | NE2 | GLN | A | 12 | 51.811 | 35.182 | 1.489 | 1.00 | 62.18 | 7 |
| | ATOM | 106 | C | GLN | A | 12 | 50.732 | 30.460 | 2.472 | 1.00 | 57.30 | 6 |
| | ATOM | 107 | O | GLN | A | 12 | 49.714 | 30.651 | 1.814 | 1.00 | 57.03 | 8 |
| | ATOM | 108 | N | THR | A | 13 | 51.029 | 29.280 | 2.987 | 1.00 | 56.84 | 7 |
| | ATOM | 109 | CA | THR | A | 13 | 50.142 | 28.147 | 2.773 | 1.00 | 57.26 | 6 |
| 60 | ATOM | 110 | CB | THR | A | 13 | 50.922 | 26.964 | 2.186 | 1.00 | 57.29 | 6 |
| | ATOM | 111 | OG1 | THR | A | 13 | 52.000 | 26.616 | 3.071 | 1.00 | 55.40 | 8 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 112 | CG2 | THR | A | 13 | 51.477 | 27.326 | 0.813 | 1.00 | 58.15 | 6 |
| | ATOM | 113 | C | THR | A | 13 | 49.411 | 27.650 | 4.013 | 1.00 | 58.45 | 6 |
| | ATOM | 114 | O | THR | A | 13 | 48.423 | 26.932 | 3.905 | 1.00 | 58.36 | 8 |
| | ATOM | 115 | N | SER | A | 14 | 49.892 | 28.034 | 5.187 | 1.00 | 60.01 | 7 |
| 5 | ATOM | 116 | CA | SER | A | 14 | 49.290 | 27.584 | 6.424 | 1.00 | 60.03 | 6 |
| | ATOM | 117 | CB | SER | A | 14 | 50.198 | 27.930 | 7.601 | 1.00 | 61.46 | 6 |
| | ATOM | 118 | OG | SER | A | 14 | 49.813 | 27.207 | 8.758 | 1.00 | 65.18 | 8 |
| | ATOM | 119 | C | SER | A | 14 | 47.899 | 28.147 | 6.664 | 1.00 | 59.50 | 6 |
| | ATOM | 120 | O | SER | A | 14 | 47.560 | 29.240 | 6.189 | 1.00 | 58.72 | 8 |
| 10 | ATOM | 121 | N | ARG | A | 15 | 47.102 | 27.377 | 7.407 | 1.00 | 58.04 | 7 |
| | ATOM | 122 | CA | ARG | A | 15 | 45.740 | 27.753 | 7.755 | 1.00 | 55.62 | 6 |
| | ATOM | 123 | CB | ARG | A | 15 | 44.744 | 26.996 | 6.877 | 1.00 | 56.74 | 6 |
| | ATOM | 124 | CG | ARG | A | 15 | 44.925 | 27.253 | 5.385 | 1.00 | 59.62 | 6 |
| | ATOM | 125 | CD | ARG | A | 15 | 43.688 | 26.851 | 4.614 | 1.00 | 61.99 | 6 |
| 15 | ATOM | 126 | NE | ARG | A | 15 | 42.519 | 27.540 | 5.151 | 1.00 | 64.02 | 7 |
| | ATOM | 127 | CZ | ARG | A | 15 | 41.261 | 27.216 | 4.870 | 1.00 | 65.48 | 6 |
| | ATOM | 128 | NH1 | ARG | A | 15 | 41.007 | 26.201 | 4.050 | 1.00 | 67.33 | 7 |
| | ATOM | 129 | NH2 | ARG | A | 15 | 40.256 | 27.908 | 5.408 | 1.00 | 64.23 | 7 |
| | ATOM | 130 | C | ARG | A | 15 | 45.516 | 27.420 | 9.219 | 1.00 | 52.12 | 6 |
| 20 | ATOM | 131 | O | ARG | A | 15 | 45.135 | 26.310 | 9.562 | 1.00 | 53.25 | 8 |
| | ATOM | 132 | N | PRO | A | 16 | 45.751 | 28.392 | 10.104 | 1.00 | 50.04 | 7 |
| | ATOM | 133 | CD | PRO | A | 16 | 46.198 | 29.750 | 9.773 | 1.00 | 48.52 | 6 |
| | ATOM | 134 | CA | PRO | A | 16 | 45.597 | 28.249 | 11.551 | 1.00 | 49.56 | 6 |
| | ATOM | 135 | CB | PRO | A | 16 | 45.959 | 29.634 | 12.073 | 1.00 | 49.66 | 6 |
| 25 | ATOM | 136 | CG | PRO | A | 16 | 46.870 | 30.165 | 11.041 | 1.00 | 49.57 | 6 |
| | ATOM | 137 | C | PRO | A | 16 | 44.215 | 27.816 | 12.016 | 1.00 | 50.11 | 6 |
| | ATOM | 138 | O | PRO | A | 16 | 44.060 | 27.322 | 13.131 | 1.00 | 51.27 | 8 |
| | ATOM | 139 | N | ASP | A | 17 | 43.208 | 28.013 | 11.176 | 1.00 | 50.70 | 7 |
| | ATOM | 140 | CA | ASP | A | 17 | 41.856 | 27.640 | 11.548 | 1.00 | 50.64 | 6 |
| 30 | ATOM | 141 | CB | ASP | A | 17 | 40.850 | 28.609 | 10.931 | 1.00 | 54.16 | 6 |
| | ATOM | 142 | CG | ASP | A | 17 | 40.873 | 29.974 | 11.592 | 1.00 | 59.76 | 6 |
| | ATOM | 143 | OD1 | ASP | A | 17 | 41.245 | 30.060 | 12.791 | 1.00 | 60.67 | 8 |
| | ATOM | 144 | OD2 | ASP | A | 17 | 40.500 | 30.965 | 10.920 | 1.00 | 62.99 | 8 |
| | ATOM | 145 | C | ASP | A | 17 | 41.482 | 26.218 | 11.157 | 1.00 | 50.71 | 6 |
| 35 | ATOM | 146 | O | ASP | A | 17 | 40.353 | 25.783 | 11.390 | 1.00 | 48.36 | 8 |
| | ATOM | 147 | N | VAL | A | 18 | 42.429 | 25.484 | 10.583 | 1.00 | 51.85 | 7 |
| | ATOM | 148 | CA | VAL | A | 18 | 42.143 | 24.128 | 10.148 | 1.00 | 52.53 | 6 |
| | ATOM | 149 | CB | VAL | A | 18 | 42.262 | 24.011 | 8.622 | 1.00 | 53.05 | 6 |
| | ATOM | 150 | CG1 | VAL | A | 18 | 41.834 | 22.618 | 8.169 | 1.00 | 51.38 | 6 |
| 40 | ATOM | 151 | CG2 | VAL | A | 18 | 41.396 | 25.077 | 7.963 | 1.00 | 51.76 | 6 |
| | ATOM | 152 | C | VAL | A | 18 | 42.993 | 23.050 | 10.779 | 1.00 | 52.56 | 6 |
| | ATOM | 153 | O | VAL | A | 18 | 44.199 | 23.006 | 10.588 | 1.00 | 52.64 | 8 |
| | ATOM | 154 | N | ILE | A | 19 | 42.327 | 22.172 | 11.519 | 1.00 | 53.41 | 7 |
| | ATOM | 155 | CA | ILE | A | 19 | 42.954 | 21.042 | 12.202 | 1.00 | 52.70 | 6 |
| 45 | ATOM | 156 | CB | ILE | A | 19 | 41.871 | 20.319 | 13.072 | 1.00 | 52.71 | 6 |
| | ATOM | 157 | CG2 | ILE | A | 19 | 40.819 | 19.671 | 12.190 | 1.00 | 52.40 | 6 |
| | ATOM | 158 | CG1 | ILE | A | 19 | 42.504 | 19.290 | 13.992 | 1.00 | 53.50 | 6 |
| | ATOM | 159 | CD1 | ILE | A | 19 | 41.546 | 18.811 | 15.056 | 1.00 | 50.39 | 6 |
| | ATOM | 160 | C | ILE | A | 19 | 43.596 | 20.097 | 11.164 | 1.00 | 52.96 | 6 |
| 50 | ATOM | 161 | O | ILE | A | 19 | 42.957 | 19.687 | 10.193 | 1.00 | 51.39 | 8 |
| | ATOM | 162 | N | PRO | A | 20 | 44.878 | 19.757 | 11.355 | 1.00 | 53.70 | 7 |
| | ATOM | 163 | CD | PRO | A | 20 | 45.711 | 20.210 | 12.472 | 1.00 | 54.14 | 6 |
| | ATOM | 164 | CA | PRO | A | 20 | 45.644 | 18.876 | 10.461 | 1.00 | 56.34 | 6 |
| | ATOM | 165 | CB | PRO | A | 20 | 47.078 | 18.996 | 10.981 | 1.00 | 56.60 | 6 |
| 55 | ATOM | 166 | CG | PRO | A | 20 | 47.060 | 20.235 | 11.840 | 1.00 | 58.05 | 6 |
| | ATOM | 167 | C | PRO | A | 20 | 45.177 | 17.432 | 10.474 | 1.00 | 58.61 | 6 |
| | ATOM | 168 | O | PRO | A | 20 | 45.974 | 16.523 | 10.682 | 1.00 | 59.22 | 8 |
| | ATOM | 169 | N | THR | A | 21 | 43.886 | 17.231 | 10.246 | 1.00 | 62.30 | 7 |
| | ATOM | 170 | CA | THR | A | 21 | 43.283 | 15.900 | 10.236 | 1.00 | 66.91 | 6 |
| 60 | ATOM | 171 | CB | THR | A | 21 | 41.765 | 16.020 | 10.495 | 1.00 | 65.83 | 6 |
| | ATOM | 172 | OG1 | THR | A | 21 | 41.516 | 15.813 | 11.883 | 1.00 | 67.19 | 8 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 173 | CG2 | THR | A | 21 | 40.975 | 15.010 | 9.687 | 1.00 | 68.42 | 6 |
| | ATOM | 174 | C | THR | A | 21 | 43.522 | 15.060 | 8.967 | 1.00 | 70.65 | 6 |
| | ATOM | 175 | O | THR | A | 21 | 43.365 | 15.538 | 7.832 | 1.00 | 70.53 | 8 |
| | ATOM | 176 | N | GLN | A | 22 | 43.899 | 13.802 | 9.179 | 1.00 | 74.54 | 7 |
| | ATOM | 177 | CA | GLN | A | 22 | 44.152 | 12.844 | 8.096 | 1.00 | 78.38 | 6 |
| 10 | ATOM | 178 | CB | GLN | A | 22 | 45.513 | 12.180 | 8.296 | 1.00 | 79.92 | 6 |
| | ATOM | 179 | CG | GLN | A | 22 | 46.668 | 13.174 | 8.402 | 1.00 | 83.40 | 6 |
| | ATOM | 180 | CD | GLN | A | 22 | 47.836 | 12.640 | 9.244 | 1.00 | 84.08 | 6 |
| | ATOM | 181 | OE1 | GLN | A | 22 | 47.709 | 12.451 | 10.467 | 1.00 | 82.79 | 8 |
| | ATOM | 182 | NE2 | GLN | A | 22 | 48.976 | 12.397 | 8.592 | 1.00 | 83.48 | 7 |
| 15 | ATOM | 183 | C | GLN | A | 22 | 43.055 | 11.779 | 8.158 | 1.00 | 80.25 | 6 |
| | ATOM | 184 | O | GLN | A | 22 | 43.050 | 10.929 | 9.058 | 1.00 | 80.25 | 8 |
| | ATOM | 185 | N | ARG | A | 23 | 42.133 | 11.825 | 7.199 | 1.00 | 82.59 | 7 |
| | ATOM | 186 | CA | ARG | A | 23 | 40.999 | 10.896 | 7.162 | 1.00 | 84.29 | 6 |
| | ATOM | 187 | CB | ARG | A | 23 | 41.478 | 9.447 | 7.095 | 1.00 | 85.05 | 6 |
| 20 | ATOM | 188 | CG | ARG | A | 23 | 41.983 | 9.032 | 5.717 | 1.00 | 87.64 | 6 |
| | ATOM | 189 | CD | ARG | A | 23 | 43.517 | 8.991 | 5.617 | 1.00 | 90.14 | 6 |
| | ATOM | 190 | NE | ARG | A | 23 | 43.958 | 8.775 | 4.231 | 1.00 | 92.92 | 7 |
| | ATOM | 191 | CZ | ARG | A | 23 | 43.557 | 7.768 | 3.447 | 1.00 | 94.10 | 6 |
| | ATOM | 192 | NH1 | ARG | A | 23 | 42.700 | 6.854 | 3.901 | 1.00 | 94.07 | 7 |
| 25 | ATOM | 193 | NH2 | ARG | A | 23 | 44.000 | 7.687 | 2.195 | 1.00 | 93.77 | 7 |
| | ATOM | 194 | C | ARG | A | 23 | 40.130 | 11.099 | 8.399 | 1.00 | 85.22 | 6 |
| | ATOM | 195 | O | ARG | A | 23 | 39.979 | 12.237 | 8.881 | 1.00 | 84.91 | 8 |
| | ATOM | 196 | N | ASP | A | 24 | 39.549 | 10.011 | 8.908 | 1.00 | 86.21 | 7 |
| | ATOM | 197 | CA | ASP | A | 24 | 38.705 | 10.105 | 10.105 | 1.00 | 86.07 | 6 |
| 30 | ATOM | 198 | CB | ASP | A | 24 | 37.689 | 8.952 | 10.194 | 1.00 | 89.13 | 6 |
| | ATOM | 199 | CG | ASP | A | 24 | 37.418 | 8.289 | 8.847 | 1.00 | 91.57 | 6 |
| | ATOM | 200 | OD1 | ASP | A | 24 | 36.945 | 8.994 | 7.900 | 1.00 | 92.21 | 8 |
| | ATOM | 201 | OD2 | ASP | A | 24 | 37.680 | 7.058 | 8.756 | 1.00 | 91.67 | 8 |
| | ATOM | 202 | C | ASP | A | 24 | 39.631 | 10.021 | 11.305 | 1.00 | 84.31 | 6 |
| 35 | ATOM | 203 | O | ASP | A | 24 | 39.173 | 9.975 | 12.458 | 1.00 | 84.64 | 8 |
| | ATOM | 204 | N | ARG | A | 25 | 40.935 | 9.981 | 11.029 | 1.00 | 81.75 | 7 |
| | ATOM | 205 | CA | ARG | A | 25 | 41.936 | 9.898 | 12.091 | 1.00 | 79.08 | 6 |
| | ATOM | 206 | CB | ARG | A | 25 | 43.309 | 9.539 | 11.527 | 1.00 | 81.87 | 6 |
| | ATOM | 207 | CG | ARG | A | 25 | 43.471 | 8.100 | 11.087 | 1.00 | 86.55 | 6 |
| 40 | ATOM | 208 | CD | ARG | A | 25 | 44.960 | 7.785 | 10.851 | 1.00 | 90.81 | 6 |
| | ATOM | 209 | NE | ARG | A | 25 | 45.187 | 6.380 | 10.489 | 1.00 | 95.61 | 7 |
| | ATOM | 210 | CZ | ARG | A | 25 | 46.388 | 5.815 | 10.345 | 1.00 | 96.85 | 6 |
| | ATOM | 211 | NH1 | ARG | A | 25 | 47.495 | 6.537 | 10.530 | 1.00 | 97.46 | 7 |
| | ATOM | 212 | NH2 | ARG | A | 25 | 46.487 | 4.522 | 10.023 | 1.00 | 97.32 | 7 |
| 45 | ATOM | 213 | C | ARG | A | 25 | 42.059 | 11.201 | 12.870 | 1.00 | 75.12 | 6 |
| | ATOM | 214 | O | ARG | A | 25 | 42.158 | 12.283 | 12.281 | 1.00 | 75.55 | 8 |
| | ATOM | 215 | N | PRO | A | 26 | 42.034 | 11.112 | 14.212 | 1.00 | 70.63 | 7 |
| | ATOM | 216 | CD | PRO | A | 26 | 41.636 | 9.933 | 14.999 | 1.00 | 69.09 | 6 |
| | ATOM | 217 | CA | PRO | A | 26 | 42.152 | 12.281 | 15.083 | 1.00 | 67.24 | 6 |
| 50 | ATOM | 218 | CB | PRO | A | 26 | 41.802 | 11.723 | 16.460 | 1.00 | 67.68 | 6 |
| | ATOM | 219 | CG | PRO | A | 26 | 40.930 | 10.565 | 16.158 | 1.00 | 68.06 | 6 |
| | ATOM | 220 | C | PRO | A | 26 | 43.593 | 12.762 | 15.053 | 1.00 | 64.53 | 6 |
| | ATOM | 221 | O | PRO | A | 26 | 44.491 | 12.000 | 14.694 | 1.00 | 63.60 | 8 |
| | ATOM | 222 | N | VAL | A | 27 | 43.816 | 14.020 | 15.420 | 1.00 | 61.16 | 7 |
| 55 | ATOM | 223 | CA | VAL | A | 27 | 45.168 | 14.544 | 15.476 | 1.00 | 57.20 | 6 |
| | ATOM | 224 | CB | VAL | A | 27 | 45.197 | 16.079 | 15.374 | 1.00 | 56.96 | 6 |
| | ATOM | 225 | CG1 | VAL | A | 27 | 46.535 | 16.615 | 15.872 | 1.00 | 54.60 | 6 |
| | ATOM | 226 | CG2 | VAL | A | 27 | 44.986 | 16.496 | 13.930 | 1.00 | 55.09 | 6 |
| | ATOM | 227 | C | VAL | A | 27 | 45.685 | 14.114 | 16.835 | 1.00 | 55.33 | 6 |
| 60 | ATOM | 228 | O | VAL | A | 27 | 45.026 | 14.328 | 17.849 | 1.00 | 53.70 | 8 |
| | ATOM | 229 | N | ALA | A | 28 | 46.852 | 13.484 | 16.858 | 1.00 | 54.55 | 7 |
| | ATOM | 230 | CA | ALA | A | 28 | 47.405 | 13.023 | 18.118 | 1.00 | 53.25 | 6 |
| | ATOM | 231 | CB | ALA | A | 28 | 48.250 | 11.785 | 17.907 | 1.00 | 52.00 | 6 |
| | ATOM | 232 | C | ALA | A | 28 | 48.230 | 14.117 | 18.761 | 1.00 | 52.77 | 6 |
| | ATOM | 233 | O | ALA | A | 28 | 49.324 | 14.451 | 18.294 | 1.00 | 52.53 | 8 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 234 | N | VAL | A | 29 | 47.683 | 14.672 | 19.837 | 1.00 | 51.33 | 7 |
| | ATOM | 235 | CA | VAL | A | 29 | 48.332 | 15.730 | 20.590 | 1.00 | 49.28 | 6 |
| | ATOM | 236 | CB | VAL | A | 29 | 47.367 | 16.921 | 20.845 | 1.00 | 47.59 | 6 |
| 5 | ATOM | 237 | CG1 | VAL | A | 29 | 48.056 | 17.985 | 21.676 | 1.00 | 44.30 | 6 |
| | ATOM | 238 | CG2 | VAL | A | 29 | 46.891 | 17.497 | 19.527 | 1.00 | 44.21 | 6 |
| | ATOM | 239 | C | VAL | A | 29 | 48.782 | 15.171 | 21.930 | 1.00 | 49.54 | 6 |
| | ATOM | 240 | O | VAL | A | 29 | 48.014 | 14.524 | 22.635 | 1.00 | 49.14 | 8 |
| | ATOM | 241 | N | SER | A | 30 | 50.043 | 15.402 | 22.261 | 1.00 | 49.54 | 7 |
| 10 | ATOM | 242 | CA | SER | A | 30 | 50.574 | 14.946 | 23.523 | 1.00 | 52.38 | 6 |
| | ATOM | 243 | CB | SER | A | 30 | 51.869 | 14.163 | 23.309 | 1.00 | 51.50 | 6 |
| | ATOM | 244 | OG | SER | A | 30 | 52.846 | 14.945 | 22.645 | 1.00 | 56.10 | 8 |
| | ATOM | 245 | C | SER | A | 30 | 50.819 | 16.187 | 24.362 | 1.00 | 54.25 | 6 |
| | ATOM | 246 | O | SER | A | 30 | 51.360 | 17.174 | 23.880 | 1.00 | 56.41 | 8 |
| 15 | ATOM | 247 | N | VAL | A | 31 | 50.396 | 16.134 | 25.618 | 1.00 | 56.86 | 7 |
| | ATOM | 248 | CA | VAL | A | 31 | 50.543 | 17.258 | 26.531 | 1.00 | 58.42 | 6 |
| | ATOM | 249 | CB | VAL | A | 31 | 49.170 | 17.768 | 27.012 | 1.00 | 58.48 | 6 |
| | ATOM | 250 | CG1 | VAL | A | 31 | 49.338 | 19.086 | 27.744 | 1.00 | 59.95 | 6 |
| | ATOM | 251 | CG2 | VAL | A | 31 | 48.219 | 17.910 | 25.835 | 1.00 | 56.73 | 6 |
| 20 | ATOM | 252 | C | VAL | A | 31 | 51.328 | 16.803 | 27.747 | 1.00 | 59.56 | 6 |
| | ATOM | 253 | O | VAL | A | 31 | 51.073 | 15.729 | 28.281 | 1.00 | 60.85 | 8 |
| | ATOM | 254 | N | SER | A | 32 | 52.271 | 17.631 | 28.185 | 1.00 | 61.06 | 7 |
| | ATOM | 255 | CA | SER | A | 32 | 53.105 | 17.312 | 29.338 | 1.00 | 60.16 | 6 |
| | ATOM | 256 | CB | SER | A | 32 | 54.388 | 16.619 | 28.868 | 1.00 | 59.88 | 6 |
| 25 | ATOM | 257 | OG | SER | A | 32 | 55.294 | 16.430 | 29.937 | 1.00 | 60.41 | 8 |
| | ATOM | 258 | C | SER | A | 32 | 53.465 | 18.568 | 30.116 | 1.00 | 60.19 | 6 |
| | ATOM | 259 | O | SER | A | 32 | 54.206 | 19.416 | 29.621 | 1.00 | 61.87 | 8 |
| | ATOM | 260 | N | LEU | A | 33 | 52.946 | 18.689 | 31.333 | 1.00 | 58.89 | 7 |
| | ATOM | 261 | CA | LEU | A | 33 | 53.256 | 19.847 | 32.170 | 1.00 | 57.23 | 6 |
| 30 | ATOM | 262 | CB | LEU | A | 33 | 52.112 | 20.142 | 33.142 | 1.00 | 55.20 | 6 |
| | ATOM | 263 | CG | LEU | A | 33 | 50.740 | 20.363 | 32.511 | 1.00 | 54.66 | 6 |
| | ATOM | 264 | CD1 | LEU | A | 33 | 49.762 | 20.880 | 33.543 | 1.00 | 51.01 | 6 |
| | ATOM | 265 | CD2 | LEU | A | 33 | 50.880 | 21.342 | 31.373 | 1.00 | 55.39 | 6 |
| | ATOM | 266 | C | LEU | A | 33 | 54.518 | 19.601 | 32.979 | 1.00 | 56.76 | 6 |
| 35 | ATOM | 267 | O | LEU | A | 33 | 54.697 | 18.526 | 33.533 | 1.00 | 58.14 | 8 |
| | ATOM | 268 | N | LYS | A | 34 | 55.394 | 20.597 | 33.028 | 1.00 | 57.17 | 7 |
| | ATOM | 269 | CA | LYS | A | 34 | 56.633 | 20.512 | 33.800 | 1.00 | 57.46 | 6 |
| | ATOM | 270 | CB | LYS | A | 34 | 57.865 | 20.690 | 32.910 | 1.00 | 60.89 | 6 |
| | ATOM | 271 | CG | LYS | A | 34 | 57.940 | 19.723 | 31.738 | 1.00 | 68.80 | 6 |
| 40 | ATOM | 272 | CD | LYS | A | 34 | 58.048 | 18.249 | 32.186 | 1.00 | 73.30 | 6 |
| | ATOM | 273 | CE | LYS | A | 34 | 58.071 | 17.290 | 30.961 | 1.00 | 74.90 | 6 |
| | ATOM | 274 | NZ | LYS | A | 34 | 58.210 | 15.842 | 31.340 | 1.00 | 75.55 | 7 |
| | ATOM | 275 | C | LYS | A | 34 | 56.522 | 21.691 | 34.741 | 1.00 | 54.81 | 6 |
| | ATOM | 276 | O | LYS | A | 34 | 56.567 | 22.834 | 34.308 | 1.00 | 55.33 | 8 |
| 45 | ATOM | 277 | N | PHE | A | 35 | 56.358 | 21.422 | 36.026 | 1.00 | 52.88 | 7 |
| | ATOM | 278 | CA | PHE | A | 35 | 56.215 | 22.507 | 36.976 | 1.00 | 50.00 | 6 |
| | ATOM | 279 | CB | PHE | A | 35 | 55.586 | 21.993 | 38.260 | 1.00 | 45.71 | 6 |
| | ATOM | 280 | CG | PHE | A | 35 | 54.186 | 21.542 | 38.072 | 1.00 | 45.07 | 6 |
| | ATOM | 281 | CD1 | PHE | A | 35 | 53.912 | 20.256 | 37.634 | 1.00 | 45.46 | 6 |
| 50 | ATOM | 282 | CD2 | PHE | A | 35 | 53.133 | 22.429 | 38.252 | 1.00 | 47.46 | 6 |
| | ATOM | 283 | CE1 | PHE | A | 35 | 52.612 | 19.848 | 37.372 | 1.00 | 45.03 | 6 |
| | ATOM | 284 | CE2 | PHE | A | 35 | 51.819 | 22.036 | 37.990 | 1.00 | 49.48 | 6 |
| | ATOM | 285 | CZ | PHE | A | 35 | 51.560 | 20.735 | 37.547 | 1.00 | 48.14 | 6 |
| | ATOM | 286 | C | PHE | A | 35 | 57.494 | 23.268 | 37.247 | 1.00 | 49.05 | 6 |
| 55 | ATOM | 287 | O | PHE | A | 35 | 58.549 | 22.687 | 37.480 | 1.00 | 48.49 | 8 |
| | ATOM | 288 | N | ILE | A | 36 | 57.374 | 24.588 | 37.191 | 1.00 | 46.86 | 7 |
| | ATOM | 289 | CA | ILE | A | 36 | 58.492 | 25.482 | 37.393 | 1.00 | 45.55 | 6 |
| | ATOM | 290 | CB | ILE | A | 36 | 58.538 | 26.551 | 36.284 | 1.00 | 43.92 | 6 |
| | ATOM | 291 | CG2 | ILE | A | 36 | 59.771 | 27.411 | 36.433 | 1.00 | 39.03 | 6 |
| 60 | ATOM | 292 | CG1 | ILE | A | 36 | 58.526 | 25.876 | 34.917 | 1.00 | 44.17 | 6 |
| | ATOM | 293 | CD1 | ILE | A | 36 | 59.671 | 24.916 | 34.699 | 1.00 | 46.33 | 6 |
| | ATOM | 294 | C | ILE | A | 36 | 58.392 | 26.181 | 38.739 | 1.00 | 46.38 | 6 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 295 | O | ILE | A | 36 | 59.405 | 26.580 | 39.318 | 1.00 | 45.40 | 8 |
| | ATOM | 296 | N | ASN | A | 37 | 57.176 | 26.340 | 39.244 | 1.00 | 46.13 | 7 |
| | ATOM | 297 | CA | ASN | A | 37 | 57.023 | 27.008 | 40.526 | 1.00 | 46.27 | 6 |
| 5 | ATOM | 298 | CB | ASN | A | 37 | 57.491 | 28.462 | 40.400 | 1.00 | 46.32 | 6 |
| | ATOM | 299 | CG | ASN | A | 37 | 58.009 | 29.030 | 41.707 | 1.00 | 48.59 | 6 |
| | ATOM | 300 | OD1 | ASN | A | 37 | 57.408 | 28.844 | 42.759 | 1.00 | 49.38 | 8 |
| | ATOM | 301 | ND2 | ASN | A | 37 | 59.124 | 29.743 | 41.639 | 1.00 | 46.71 | 7 |
| | ATOM | 302 | C | ASN | A | 37 | 55.595 | 26.975 | 41.046 | 1.00 | 46.17 | 6 |
| 10 | ATOM | 303 | O | ASN | A | 37 | 54.644 | 26.799 | 40.281 | 1.00 | 44.02 | 8 |
| | ATOM | 304 | N | ILE | A | 38 | 55.465 | 27.117 | 42.362 | 1.00 | 46.64 | 7 |
| | ATOM | 305 | CA | ILE | A | 38 | 54.173 | 27.158 | 43.033 | 1.00 | 48.46 | 6 |
| | ATOM | 306 | CB | ILE | A | 38 | 53.988 | 25.951 | 43.923 | 1.00 | 47.34 | 6 |
| | ATOM | 307 | CG2 | ILE | A | 38 | 52.680 | 26.066 | 44.671 | 1.00 | 49.13 | 6 |
| | ATOM | 308 | CG1 | ILE | A | 38 | 53.983 | 24.697 | 43.050 | 1.00 | 48.40 | 6 |
| 15 | ATOM | 309 | CD1 | ILE | A | 38 | 54.079 | 23.402 | 43.791 | 1.00 | 47.55 | 6 |
| | ATOM | 310 | C | ILE | A | 38 | 54.245 | 28.433 | 43.847 | 1.00 | 50.74 | 6 |
| | ATOM | 311 | O | ILE | A | 38 | 54.979 | 28.505 | 44.817 | 1.00 | 53.13 | 8 |
| | ATOM | 312 | N | LEU | A | 39 | 53.485 | 29.438 | 43.433 | 1.00 | 53.46 | 7 |
| 20 | ATOM | 313 | CA | LEU | A | 39 | 53.527 | 30.757 | 44.045 | 1.00 | 55.16 | 6 |
| | ATOM | 314 | CB | LEU | A | 39 | 53.350 | 31.806 | 42.952 | 1.00 | 54.91 | 6 |
| | ATOM | 315 | CG | LEU | A | 39 | 54.330 | 31.591 | 41.800 | 1.00 | 57.26 | 6 |
| | ATOM | 316 | CD1 | LEU | A | 39 | 54.108 | 32.647 | 40.728 | 1.00 | 54.71 | 6 |
| | ATOM | 317 | CD2 | LEU | A | 39 | 55.757 | 31.623 | 42.341 | 1.00 | 54.68 | 6 |
| 25 | ATOM | 318 | C | LEU | A | 39 | 52.613 | 31.098 | 45.203 | 1.00 | 56.69 | 6 |
| | ATOM | 319 | O | LEU | A | 39 | 53.043 | 31.750 | 46.157 | 1.00 | 59.24 | 8 |
| | ATOM | 320 | N | GLU | A | 40 | 51.352 | 30.715 | 45.123 | 1.00 | 56.60 | 7 |
| | ATOM | 321 | CA | GLU | A | 40 | 50.451 | 31.019 | 46.216 | 1.00 | 58.75 | 6 |
| | ATOM | 322 | CB | GLU | A | 40 | 49.617 | 32.251 | 45.920 | 1.00 | 59.61 | 6 |
| 30 | ATOM | 323 | CG | GLU | A | 40 | 50.426 | 33.520 | 45.821 | 1.00 | 65.69 | 6 |
| | ATOM | 324 | CD | GLU | A | 40 | 49.547 | 34.752 | 45.683 | 1.00 | 69.26 | 6 |
| | ATOM | 325 | OE1 | GLU | A | 40 | 48.747 | 34.812 | 44.715 | 1.00 | 72.53 | 8 |
| | ATOM | 326 | OE2 | GLU | A | 40 | 49.655 | 35.659 | 46.543 | 1.00 | 69.31 | 8 |
| | ATOM | 327 | C | GLU | A | 40 | 49.534 | 29.863 | 46.448 | 1.00 | 60.49 | 6 |
| | ATOM | 328 | O | GLU | A | 40 | 49.006 | 29.275 | 45.509 | 1.00 | 62.83 | 8 |
| 35 | ATOM | 329 | N | VAL | A | 41 | 49.348 | 29.525 | 47.710 | 1.00 | 60.13 | 7 |
| | ATOM | 330 | CA | VAL | A | 41 | 48.474 | 28.431 | 48.049 | 1.00 | 60.14 | 6 |
| | ATOM | 331 | CB | VAL | A | 41 | 49.292 | 27.230 | 48.576 | 1.00 | 59.98 | 6 |
| | ATOM | 332 | CG1 | VAL | A | 41 | 48.376 | 26.185 | 49.146 | 1.00 | 59.73 | 6 |
| 40 | ATOM | 333 | CG2 | VAL | A | 41 | 50.118 | 26.632 | 47.444 | 1.00 | 59.26 | 6 |
| | ATOM | 334 | C | VAL | A | 41 | 47.510 | 28.934 | 49.109 | 1.00 | 60.58 | 6 |
| | ATOM | 335 | O | VAL | A | 41 | 47.864 | 29.793 | 49.934 | 1.00 | 61.24 | 8 |
| | ATOM | 336 | N | ASN | A | 42 | 46.283 | 28.428 | 49.059 | 1.00 | 59.54 | 7 |
| | ATOM | 337 | CA | ASN | A | 42 | 45.267 | 28.806 | 50.024 | 1.00 | 60.72 | 6 |
| | ATOM | 338 | CB | ASN | A | 42 | 44.346 | 29.895 | 49.463 | 1.00 | 59.36 | 6 |
| 45 | ATOM | 339 | CG | ASN | A | 42 | 43.473 | 30.530 | 50.533 | 1.00 | 59.07 | 6 |
| | ATOM | 340 | OD1 | ASN | A | 42 | 42.811 | 29.835 | 51.303 | 1.00 | 60.43 | 8 |
| | ATOM | 341 | ND2 | ASN | A | 42 | 43.462 | 31.856 | 50.582 | 1.00 | 57.17 | 7 |
| | ATOM | 342 | C | ASN | A | 42 | 44.474 | 27.535 | 50.286 | 1.00 | 62.57 | 6 |
| 50 | ATOM | 343 | O | ASN | A | 42 | 43.654 | 27.107 | 49.460 | 1.00 | 62.42 | 8 |
| | ATOM | 344 | N | GLU | A | 43 | 44.731 | 26.921 | 51.435 | 1.00 | 63.02 | 7 |
| | ATOM | 345 | CA | GLU | A | 43 | 44.045 | 25.695 | 51.792 | 1.00 | 62.62 | 6 |
| | ATOM | 346 | CB | GLU | A | 43 | 44.772 | 25.004 | 52.942 | 1.00 | 65.20 | 6 |
| | ATOM | 347 | CG | GLU | A | 43 | 44.206 | 23.642 | 53.253 | 1.00 | 67.62 | 6 |
| | ATOM | 348 | CD | GLU | A | 43 | 45.088 | 22.827 | 54.174 | 1.00 | 69.40 | 6 |
| 55 | ATOM | 349 | OE1 | GLU | A | 43 | 44.628 | 21.739 | 54.581 | 1.00 | 71.48 | 8 |
| | ATOM | 350 | OE2 | GLU | A | 43 | 46.228 | 23.256 | 54.479 | 1.00 | 67.83 | 8 |
| | ATOM | 351 | C | GLU | A | 43 | 42.595 | 25.959 | 52.169 | 1.00 | 61.53 | 6 |
| | ATOM | 352 | O | GLU | A | 43 | 41.755 | 25.058 | 52.086 | 1.00 | 59.68 | 8 |
| 60 | ATOM | 353 | N | ILE | A | 44 | 42.309 | 27.197 | 52.575 | 1.00 | 60.06 | 7 |
| | ATOM | 354 | CA | ILE | A | 44 | 40.957 | 27.580 | 52.951 | 1.00 | 60.59 | 6 |
| | ATOM | 355 | CB | ILE | A | 44 | 40.923 | 28.953 | 53.632 | 1.00 | 60.98 | 6 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 356 | CG2 | ILE | A | 44 | 39.469 | 29.343 | 53.943 | 1.00 | 61.06 | 6 |
| | ATOM | 357 | CG1 | ILE | A | 44 | 41.749 | 28.921 | 54.918 | 1.00 | 61.51 | 6 |
| | ATOM | 358 | CD1 | ILE | A | 44 | 41.119 | 28.117 | 56.022 | 1.00 | 61.37 | 6 |
| | ATOM | 359 | C | ILE | A | 44 | 40.069 | 27.660 | 51.718 | 1.00 | 61.06 | 6 |
| 5 | ATOM | 360 | O | ILE | A | 44 | 38.942 | 27.148 | 51.708 | 1.00 | 61.53 | 8 |
| | ATOM | 361 | N | THR | A | 45 | 40.581 | 28.302 | 50.674 | 1.00 | 60.25 | 7 |
| | ATOM | 362 | CA | THR | A | 45 | 39.826 | 28.464 | 49.426 | 1.00 | 58.34 | 6 |
| | ATOM | 363 | CB | THR | A | 45 | 40.086 | 29.844 | 48.805 | 1.00 | 58.12 | 6 |
| 10 | ATOM | 364 | OG1 | THR | A | 45 | 41.492 | 29.992 | 48.535 | 1.00 | 58.85 | 8 |
| | ATOM | 365 | CG2 | THR | A | 45 | 39.632 | 30.934 | 49.762 | 1.00 | 56.98 | 6 |
| | ATOM | 366 | C | THR | A | 45 | 40.139 | 27.407 | 48.374 | 1.00 | 56.43 | 6 |
| | ATOM | 367 | O | THR | A | 45 | 39.465 | 27.328 | 47.349 | 1.00 | 54.64 | 8 |
| | ATOM | 368 | N | ASN | A | 46 | 41.169 | 26.607 | 48.620 | 1.00 | 55.73 | 7 |
| | ATOM | 369 | CA | ASN | A | 46 | 41.534 | 25.563 | 47.677 | 1.00 | 56.27 | 6 |
| 15 | ATOM | 370 | CB | ASN | A | 46 | 40.390 | 24.557 | 47.560 | 1.00 | 55.82 | 6 |
| | ATOM | 371 | CG | ASN | A | 46 | 40.612 | 23.327 | 48.412 | 1.00 | 56.92 | 6 |
| | ATOM | 372 | OD1 | ASN | A | 46 | 39.671 | 22.621 | 48.746 | 1.00 | 55.85 | 8 |
| | ATOM | 373 | ND2 | ASN | A | 46 | 41.866 | 23.058 | 48.754 | 1.00 | 54.55 | 7 |
| 20 | ATOM | 374 | C | ASN | A | 46 | 41.869 | 26.127 | 46.299 | 1.00 | 56.62 | 6 |
| | ATOM | 375 | O | ASN | A | 46 | 41.350 | 25.659 | 45.283 | 1.00 | 58.80 | 8 |
| | ATOM | 376 | N | GLU | A | 47 | 42.744 | 27.130 | 46.275 | 1.00 | 54.91 | 7 |
| | ATOM | 377 | CA | GLU | A | 47 | 43.156 | 27.766 | 45.044 | 1.00 | 52.39 | 6 |
| | ATOM | 378 | CB | GLU | A | 47 | 42.606 | 29.183 | 44.999 | 1.00 | 50.63 | 6 |
| 25 | ATOM | 379 | CG | GLU | A | 47 | 41.107 | 29.247 | 44.938 | 1.00 | 48.77 | 6 |
| | ATOM | 380 | CD | GLU | A | 47 | 40.601 | 30.675 | 44.951 | 1.00 | 53.28 | 6 |
| | ATOM | 381 | OE1 | GLU | A | 47 | 41.370 | 31.577 | 44.568 | 1.00 | 51.68 | 8 |
| | ATOM | 382 | OE2 | GLU | A | 47 | 39.429 | 30.902 | 45.333 | 1.00 | 58.43 | 8 |
| | ATOM | 383 | C | GLU | A | 47 | 44.671 | 27.776 | 44.979 | 1.00 | 52.87 | 6 |
| 30 | ATOM | 384 | O | GLU | A | 47 | 45.347 | 28.009 | 45.981 | 1.00 | 53.20 | 8 |
| | ATOM | 385 | N | VAL | A | 48 | 45.208 | 27.513 | 43.797 | 1.00 | 53.53 | 7 |
| | ATOM | 386 | CA | VAL | A | 48 | 46.656 | 27.481 | 43.619 | 1.00 | 53.36 | 6 |
| | ATOM | 387 | CB | VAL | A | 48 | 47.147 | 26.043 | 43.318 | 1.00 | 53.31 | 6 |
| | ATOM | 388 | CG1 | VAL | A | 48 | 48.646 | 26.029 | 43.122 | 1.00 | 55.73 | 6 |
| | ATOM | 389 | CG2 | VAL | A | 48 | 46.781 | 25.130 | 44.456 | 1.00 | 52.72 | 6 |
| 35 | ATOM | 390 | C | VAL | A | 48 | 47.108 | 28.390 | 42.484 | 1.00 | 52.90 | 6 |
| | ATOM | 391 | O | VAL | A | 48 | 46.441 | 28.504 | 41.454 | 1.00 | 54.54 | 8 |
| | ATOM | 392 | N | ASP | A | 49 | 48.242 | 29.046 | 42.691 | 1.00 | 52.21 | 7 |
| | ATOM | 393 | CA | ASP | A | 49 | 48.818 | 29.928 | 41.692 | 1.00 | 51.57 | 6 |
| 40 | ATOM | 394 | CB | ASP | A | 49 | 49.084 | 31.291 | 42.304 | 1.00 | 52.64 | 6 |
| | ATOM | 395 | CG | ASP | A | 49 | 49.264 | 32.352 | 41.268 | 1.00 | 53.86 | 6 |
| | ATOM | 396 | OD1 | ASP | A | 49 | 49.900 | 32.051 | 40.246 | 1.00 | 54.56 | 8 |
| | ATOM | 397 | OD2 | ASP | A | 49 | 48.779 | 33.482 | 41.474 | 1.00 | 57.00 | 8 |
| | ATOM | 398 | C | ASP | A | 49 | 50.121 | 29.241 | 41.313 | 1.00 | 50.45 | 6 |
| 45 | ATOM | 399 | O | ASP | A | 49 | 51.074 | 29.254 | 42.075 | 1.00 | 52.15 | 8 |
| | ATOM | 400 | N | VAL | A | 50 | 50.155 | 28.636 | 40.135 | 1.00 | 49.83 | 7 |
| | ATOM | 401 | CA | VAL | A | 50 | 51.329 | 27.893 | 39.711 | 1.00 | 49.77 | 6 |
| | ATOM | 402 | CB | VAL | A | 50 | 50.992 | 26.372 | 39.723 | 1.00 | 51.61 | 6 |
| | ATOM | 403 | CG1 | VAL | A | 50 | 50.095 | 26.015 | 38.531 | 1.00 | 51.90 | 6 |
| 50 | ATOM | 404 | CG2 | VAL | A | 50 | 52.265 | 25.539 | 39.721 | 1.00 | 53.03 | 6 |
| | ATOM | 405 | C | VAL | A | 50 | 51.890 | 28.290 | 38.335 | 1.00 | 49.01 | 6 |
| | ATOM | 406 | O | VAL | A | 50 | 51.193 | 28.878 | 37.508 | 1.00 | 50.33 | 8 |
| | ATOM | 407 | N | VAL | A | 51 | 53.163 | 27.974 | 38.117 | 1.00 | 46.39 | 7 |
| | ATOM | 408 | CA | VAL | A | 51 | 53.863 | 28.245 | 36.861 | 1.00 | 45.41 | 6 |
| | ATOM | 409 | CB | VAL | A | 51 | 55.111 | 29.134 | 37.083 | 1.00 | 43.93 | 6 |
| 55 | ATOM | 410 | CG1 | VAL | A | 51 | 55.943 | 29.182 | 35.807 | 1.00 | 42.09 | 6 |
| | ATOM | 411 | CG2 | VAL | A | 51 | 54.696 | 30.536 | 37.497 | 1.00 | 41.05 | 6 |
| | ATOM | 412 | C | VAL | A | 51 | 54.336 | 26.899 | 36.291 | 1.00 | 46.83 | 6 |
| | ATOM | 413 | O | VAL | A | 51 | 54.879 | 26.063 | 37.016 | 1.00 | 47.95 | 8 |
| 60 | ATOM | 414 | N | PHE | A | 52 | 54.147 | 26.684 | 34.996 | 1.00 | 45.38 | 7 |
| | ATOM | 415 | CA | PHE | A | 52 | 54.560 | 25.423 | 34.402 | 1.00 | 44.58 | 6 |
| | ATOM | 416 | CB | PHE | A | 52 | 53.485 | 24.373 | 34.662 | 1.00 | 44.09 | 6 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 417 | CG | PHE | A | 52 | 52.155 | 24.718 | 34.068 | 1.00 | 43.27 | 6 |
| | ATOM | 418 | CD1 | PHE | A | 52 | 51.857 | 24.393 | 32.758 | 1.00 | 42.79 | 6 |
| | ATOM | 419 | CD2 | PHE | A | 52 | 51.211 | 25.411 | 34.805 | 1.00 | 45.35 | 6 |
| | ATOM | 420 | CE1 | PHE | A | 52 | 50.643 | 24.755 | 32.194 | 1.00 | 41.86 | 6 |
| 5 | ATOM | 421 | CE2 | PHE | A | 52 | 49.991 | 25.776 | 34.240 | 1.00 | 45.03 | 6 |
| | ATOM | 422 | CZ | PHE | A | 52 | 49.712 | 25.445 | 32.933 | 1.00 | 41.04 | 6 |
| | ATOM | 423 | C | PHE | A | 52 | 54.789 | 25.547 | 32.906 | 1.00 | 45.52 | 6 |
| | ATOM | 424 | O | PHE | A | 52 | 54.403 | 26.536 | 32.288 | 1.00 | 46.49 | 8 |
| | ATOM | 425 | N | TRP | A | 53 | 55.431 | 24.541 | 32.328 | 1.00 | 45.07 | 7 |
| 10 | ATOM | 426 | CA | TRP | A | 53 | 55.662 | 24.527 | 30.898 | 1.00 | 46.61 | 6 |
| | ATOM | 427 | CB | TRP | A | 53 | 57.043 | 24.000 | 30.573 | 1.00 | 48.36 | 6 |
| | ATOM | 428 | CG | TRP | A | 53 | 58.137 | 24.899 | 30.983 | 1.00 | 50.29 | 6 |
| | ATOM | 429 | CD2 | TRP | A | 53 | 59.531 | 24.604 | 30.942 | 1.00 | 50.34 | 6 |
| | ATOM | 430 | CE2 | TRP | A | 53 | 60.213 | 25.755 | 31.386 | 1.00 | 51.89 | 6 |
| 15 | ATOM | 431 | CE3 | TRP | A | 53 | 60.274 | 23.473 | 30.570 | 1.00 | 52.05 | 6 |
| | ATOM | 432 | CD1 | TRP | A | 53 | 58.024 | 26.175 | 31.436 | 1.00 | 50.84 | 6 |
| | ATOM | 433 | NE1 | TRP | A | 53 | 59.267 | 26.700 | 31.682 | 1.00 | 52.12 | 7 |
| | ATOM | 434 | CZ2 | TRP | A | 53 | 61.605 | 25.817 | 31.470 | 1.00 | 53.79 | 6 |
| | ATOM | 435 | CZ3 | TRP | A | 53 | 61.660 | 23.527 | 30.649 | 1.00 | 53.82 | 6 |
| 20 | ATOM | 436 | CH2 | TRP | A | 53 | 62.314 | 24.697 | 31.099 | 1.00 | 55.14 | 6 |
| | ATOM | 437 | C | TRP | A | 53 | 54.644 | 23.599 | 30.285 | 1.00 | 47.55 | 6 |
| | ATOM | 438 | O | TRP | A | 53 | 54.645 | 22.410 | 30.564 | 1.00 | 49.29 | 8 |
| | ATOM | 439 | N | GLN | A | 54 | 53.765 | 24.139 | 29.457 | 1.00 | 47.91 | 7 |
| | ATOM | 440 | CA | GLN | A | 54 | 52.765 | 23.312 | 28.825 | 1.00 | 48.38 | 6 |
| 25 | ATOM | 441 | CB | GLN | A | 54 | 51.517 | 24.132 | 28.529 | 1.00 | 47.98 | 6 |
| | ATOM | 442 | CG | GLN | A | 54 | 50.322 | 23.309 | 28.095 | 1.00 | 50.36 | 6 |
| | ATOM | 443 | CD | GLN | A | 54 | 49.001 | 24.016 | 28.375 | 1.00 | 54.00 | 6 |
| | ATOM | 444 | OE1 | GLN | A | 54 | 48.697 | 24.360 | 29.515 | 1.00 | 53.48 | 8 |
| | ATOM | 445 | NE2 | GLN | A | 54 | 48.209 | 24.231 | 27.335 | 1.00 | 57.12 | 7 |
| 30 | ATOM | 446 | C | GLN | A | 54 | 53.378 | 22.755 | 27.555 | 1.00 | 49.13 | 6 |
| | ATOM | 447 | O | GLN | A | 54 | 53.095 | 23.203 | 26.453 | 1.00 | 50.86 | 8 |
| | ATOM | 448 | N | GLN | A | 55 | 54.251 | 21.779 | 27.738 | 1.00 | 50.50 | 7 |
| | ATOM | 449 | CA | GLN | A | 55 | 54.937 | 21.122 | 26.641 | 1.00 | 52.90 | 6 |
| | ATOM | 450 | CB | GLN | A | 55 | 55.995 | 20.200 | 27.234 | 1.00 | 58.12 | 6 |
| 35 | ATOM | 451 | CG | GLN | A | 55 | 56.699 | 19.288 | 26.263 | 1.00 | 66.05 | 6 |
| | ATOM | 452 | CD | GLN | A | 55 | 57.909 | 18.634 | 26.907 | 1.00 | 71.07 | 6 |
| | ATOM | 453 | OE1 | GLN | A | 55 | 57.890 | 18.307 | 28.107 | 1.00 | 73.93 | 8 |
| | ATOM | 454 | NE2 | GLN | A | 55 | 58.969 | 18.442 | 26.123 | 1.00 | 72.99 | 7 |
| | ATOM | 455 | C | GLN | A | 55 | 53.939 | 20.353 | 25.774 | 1.00 | 51.30 | 6 |
| 40 | ATOM | 456 | O | GLN | A | 55 | 53.451 | 19.293 | 26.151 | 1.00 | 50.67 | 8 |
| | ATOM | 457 | N | THR | A | 56 | 53.648 | 20.907 | 24.604 | 1.00 | 49.14 | 7 |
| | ATOM | 458 | CA | THR | A | 56 | 52.690 | 20.325 | 23.684 | 1.00 | 46.69 | 6 |
| | ATOM | 459 | CB | THR | A | 56 | 51.597 | 21.347 | 23.342 | 1.00 | 45.67 | 6 |
| | ATOM | 460 | OG1 | THR | A | 56 | 51.138 | 21.969 | 24.541 | 1.00 | 45.84 | 8 |
| 45 | ATOM | 461 | CG2 | THR | A | 56 | 50.426 | 20.673 | 22.666 | 1.00 | 45.93 | 6 |
| | ATOM | 462 | C | THR | A | 56 | 53.344 | 19.878 | 22.389 | 1.00 | 46.05 | 6 |
| | ATOM | 463 | O | THR | A | 56 | 54.286 | 20.503 | 21.917 | 1.00 | 46.13 | 8 |
| | ATOM | 464 | N | THR | A | 57 | 52.836 | 18.796 | 21.812 | 1.00 | 44.22 | 7 |
| | ATOM | 465 | CA | THR | A | 57 | 53.384 | 18.286 | 20.569 | 1.00 | 44.65 | 6 |
| 50 | ATOM | 466 | CB | THR | A | 57 | 54.511 | 17.270 | 20.823 | 1.00 | 44.59 | 6 |
| | ATOM | 467 | OG1 | THR | A | 57 | 55.593 | 17.914 | 21.499 | 1.00 | 42.38 | 8 |
| | ATOM | 468 | CG2 | THR | A | 57 | 55.036 | 16.733 | 19.512 | 1.00 | 49.11 | 6 |
| | ATOM | 469 | C | THR | A | 57 | 52.316 | 17.627 | 19.721 | 1.00 | 43.97 | 6 |
| | ATOM | 470 | O | THR | A | 57 | 51.377 | 17.039 | 20.239 | 1.00 | 44.62 | 8 |
| 55 | ATOM | 471 | N | TRP | A | 58 | 52.452 | 17.753 | 18.410 | 1.00 | 42.72 | 7 |
| | ATOM | 472 | CA | TRP | A | 58 | 51.502 | 17.153 | 17.489 | 1.00 | 44.75 | 6 |
| | ATOM | 473 | CB | TRP | A | 58 | 50.139 | 17.883 | 17.529 | 1.00 | 42.24 | 6 |
| | ATOM | 474 | CG | TRP | A | 58 | 50.130 | 19.267 | 16.967 | 1.00 | 40.43 | 6 |
| | ATOM | 475 | CD2 | TRP | A | 58 | 50.427 | 20.473 | 17.668 | 1.00 | 39.55 | 6 |
| 60 | ATOM | 476 | CE2 | TRP | A | 58 | 50.354 | 21.521 | 16.735 | 1.00 | 41.08 | 6 |
| | ATOM | 477 | CE3 | TRP | A | 58 | 50.755 | 20.770 | 18.995 | 1.00 | 36.98 | 6 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 478 | CD1 | TRP | A | 58 | 49.887 | 19.624 | 15.677 | 1.00 | 39.98 | 6 |
| | ATOM | 479 | NE1 | TRP | A | 58 | 50.019 | 20.971 | 15.527 | 1.00 | 41.55 | 7 |
| | ATOM | 480 | CZ2 | TRP | A | 58 | 50.599 | 22.850 | 17.084 | 1.00 | 40.32 | 6 |
| | ATOM | 481 | CZ3 | TRP | A | 58 | 50.997 | 22.081 | 19.341 | 1.00 | 37.03 | 6 |
| | ATOM | 482 | CH2 | TRP | A | 58 | 50.919 | 23.109 | 18.389 | 1.00 | 38.53 | 6 |
| 10 | ATOM | 483 | C | TRP | A | 58 | 52.112 | 17.184 | 16.098 | 1.00 | 47.09 | 6 |
| | ATOM | 484 | O | TRP | A | 58 | 53.226 | 17.675 | 15.915 | 1.00 | 47.06 | 8 |
| | ATOM | 485 | N | SER | A | 59 | 51.390 | 16.670 | 15.115 | 1.00 | 48.64 | 7 |
| | ATOM | 486 | CA | SER | A | 59 | 51.933 | 16.631 | 13.782 | 1.00 | 50.92 | 6 |
| | ATOM | 487 | CB | SER | A | 59 | 52.245 | 15.187 | 13.435 | 1.00 | 53.25 | 6 |
| 15 | ATOM | 488 | OG | SER | A | 59 | 53.191 | 15.109 | 12.389 | 1.00 | 62.80 | 8 |
| | ATOM | 489 | C | SER | A | 59 | 51.020 | 17.229 | 12.735 | 1.00 | 52.80 | 6 |
| | ATOM | 490 | O | SER | A | 59 | 49.828 | 16.942 | 12.696 | 1.00 | 53.05 | 8 |
| | ATOM | 491 | N | ASP | A | 60 | 51.602 | 18.065 | 11.881 | 1.00 | 55.45 | 7 |
| | ATOM | 492 | CA | ASP | A | 60 | 50.881 | 18.721 | 10.792 | 1.00 | 57.44 | 6 |
| 20 | ATOM | 493 | CB | ASP | A | 60 | 50.741 | 20.221 | 11.071 | 1.00 | 57.33 | 6 |
| | ATOM | 494 | CG | ASP | A | 60 | 49.856 | 20.936 | 10.058 | 1.00 | 57.43 | 6 |
| | ATOM | 495 | OD1 | ASP | A | 60 | 49.776 | 20.486 | 8.896 | 1.00 | 57.47 | 8 |
| | ATOM | 496 | OD2 | ASP | A | 60 | 49.256 | 21.967 | 10.424 | 1.00 | 56.76 | 8 |
| | ATOM | 497 | C | ASP | A | 60 | 51.726 | 18.510 | 9.541 | 1.00 | 59.20 | 6 |
| 25 | ATOM | 498 | O | ASP | A | 60 | 52.679 | 19.245 | 9.304 | 1.00 | 58.82 | 8 |
| | ATOM | 499 | N | ARG | A | 61 | 51.372 | 17.503 | 8.748 | 1.00 | 61.30 | 7 |
| | ATOM | 500 | CA | ARG | A | 61 | 52.115 | 17.181 | 7.533 | 1.00 | 63.09 | 6 |
| | ATOM | 501 | CB | ARG | A | 61 | 51.643 | 15.845 | 6.958 | 1.00 | 67.23 | 6 |
| | ATOM | 502 | CG | ARG | A | 61 | 52.191 | 14.594 | 7.653 | 1.00 | 72.92 | 6 |
| 30 | ATOM | 503 | CD | ARG | A | 61 | 51.883 | 13.355 | 6.786 | 1.00 | 81.01 | 6 |
| | ATOM | 504 | NE | ARG | A | 61 | 52.441 | 12.091 | 7.291 | 1.00 | 85.79 | 7 |
| | ATOM | 505 | CZ | ARG | A | 61 | 52.320 | 10.917 | 6.660 | 1.00 | 87.50 | 6 |
| | ATOM | 506 | NH1 | ARG | A | 61 | 51.665 | 10.843 | 5.501 | 1.00 | 88.31 | 7 |
| | ATOM | 507 | NH2 | ARG | A | 61 | 52.852 | 9.815 | 7.179 | 1.00 | 87.74 | 7 |
| 35 | ATOM | 508 | C | ARG | A | 61 | 52.073 | 18.238 | 6.430 | 1.00 | 61.94 | 6 |
| | ATOM | 509 | O | ARG | A | 61 | 52.927 | 18.225 | 5.550 | 1.00 | 61.39 | 8 |
| | ATOM | 510 | N | THR | A | 62 | 51.095 | 19.141 | 6.461 | 1.00 | 60.78 | 7 |
| | ATOM | 511 | CA | THR | A | 62 | 51.017 | 20.175 | 5.434 | 1.00 | 59.76 | 6 |
| | ATOM | 512 | CB | THR | A | 62 | 49.666 | 20.952 | 5.483 | 1.00 | 60.01 | 6 |
| 40 | ATOM | 513 | OG1 | THR | A | 62 | 49.582 | 21.720 | 6.689 | 1.00 | 62.71 | 8 |
| | ATOM | 514 | CG2 | THR | A | 62 | 48.500 | 20.000 | 5.442 | 1.00 | 59.86 | 6 |
| | ATOM | 515 | C | THR | A | 62 | 52.172 | 21.171 | 5.616 | 1.00 | 58.73 | 6 |
| | ATOM | 516 | O | THR | A | 62 | 52.400 | 22.044 | 4.774 | 1.00 | 59.33 | 8 |
| | ATOM | 517 | N | LEU | A | 63 | 52.898 | 21.031 | 6.720 | 1.00 | 56.50 | 7 |
| 45 | ATOM | 518 | CA | LEU | A | 63 | 54.029 | 21.903 | 7.020 | 1.00 | 55.97 | 6 |
| | ATOM | 519 | CB | LEU | A | 63 | 54.088 | 22.205 | 8.521 | 1.00 | 53.19 | 6 |
| | ATOM | 520 | CG | LEU | A | 63 | 52.866 | 22.837 | 9.174 | 1.00 | 52.76 | 6 |
| | ATOM | 521 | CD1 | LEU | A | 63 | 53.074 | 22.909 | 10.672 | 1.00 | 51.73 | 6 |
| | ATOM | 522 | CD2 | LEU | A | 63 | 52.629 | 24.217 | 8.589 | 1.00 | 53.34 | 6 |
| 50 | ATOM | 523 | C | LEU | A | 63 | 55.351 | 21.264 | 6.603 | 1.00 | 55.80 | 6 |
| | ATOM | 524 | O | LEU | A | 63 | 56.366 | 21.947 | 6.509 | 1.00 | 54.36 | 8 |
| | ATOM | 525 | N | ALA | A | 64 | 55.332 | 19.952 | 6.368 | 1.00 | 56.30 | 7 |
| | ATOM | 526 | CA | ALA | A | 64 | 56.532 | 19.207 | 5.987 | 1.00 | 56.99 | 6 |
| | ATOM | 527 | CB | ALA | A | 64 | 56.194 | 17.744 | 5.810 | 1.00 | 54.20 | 6 |
| 55 | ATOM | 528 | C | ALA | A | 64 | 57.176 | 19.745 | 4.715 | 1.00 | 59.20 | 6 |
| | ATOM | 529 | O | ALA | A | 64 | 56.487 | 20.224 | 3.816 | 1.00 | 60.08 | 8 |
| | ATOM | 530 | N | TRP | A | 65 | 58.502 | 19.646 | 4.651 | 1.00 | 60.65 | 7 |
| | ATOM | 531 | CA | TRP | A | 65 | 59.295 | 20.104 | 3.506 | 1.00 | 62.47 | 6 |
| | ATOM | 532 | CB | TRP | A | 65 | 59.623 | 21.588 | 3.667 | 1.00 | 59.37 | 6 |
| 60 | ATOM | 533 | CG | TRP | A | 65 | 60.773 | 21.870 | 4.613 | 1.00 | 56.94 | 6 |
| | ATOM | 534 | CD2 | TRP | A | 65 | 60.685 | 22.167 | 6.020 | 1.00 | 56.89 | 6 |
| | ATOM | 535 | CE2 | TRP | A | 65 | 62.001 | 22.424 | 6.475 | 1.00 | 55.08 | 6 |
| | ATOM | 536 | CE3 | TRP | A | 65 | 59.622 | 22.245 | 6.938 | 1.00 | 54.01 | 6 |
| | ATOM | 537 | CD1 | TRP | A | 65 | 62.097 | 21.947 | 4.292 | 1.00 | 55.45 | 6 |
| | ATOM | 538 | NE1 | TRP | A | 65 | 62.838 | 22.282 | 5.400 | 1.00 | 53.98 | 7 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 539 | CZ2 | TRP | A | 65 | 62.286 | 22.757 | 7.808 | 1.00 | 52.03 | 6 |
| | ATOM | 540 | CZ3 | TRP | A | 65 | 59.910 | 22.577 | 8.266 | 1.00 | 53.82 | 6 |
| | ATOM | 541 | CH2 | TRP | A | 65 | 61.232 | 22.829 | 8.684 | 1.00 | 51.71 | 6 |
| | ATOM | 542 | C | TRP | A | 65 | 60.603 | 19.297 | 3.445 | 1.00 | 65.72 | 6 |
| 5 | ATOM | 543 | O | TRP | A | 65 | 61.091 | 18.825 | 4.479 | 1.00 | 66.89 | 8 |
| | ATOM | 544 | N | ASN | A | 66 | 61.181 | 19.138 | 2.255 | 1.00 | 68.69 | 7 |
| | ATOM | 545 | CA | ASN | A | 66 | 62.431 | 18.371 | 2.149 | 1.00 | 71.84 | 6 |
| | ATOM | 546 | CB | ASN | A | 66 | 62.735 | 17.983 | 0.689 | 1.00 | 73.23 | 6 |
| | ATOM | 547 | CG | ASN | A | 66 | 63.968 | 17.084 | 0.568 | 1.00 | 76.18 | 6 |
| 10 | ATOM | 548 | OD1 | ASN | A | 66 | 64.473 | 16.822 | -0.541 | 1.00 | 76.68 | 8 |
| | ATOM | 549 | ND2 | ASN | A | 66 | 64.463 | 16.606 | 1.715 | 1.00 | 76.39 | 7 |
| | ATOM | 550 | C | ASN | A | 66 | 63.581 | 19.199 | 2.723 | 1.00 | 71.96 | 6 |
| | ATOM | 551 | O | ASN | A | 66 | 63.902 | 20.279 | 2.217 | 1.00 | 72.02 | 8 |
| | ATOM | 552 | N | SER | A | 67 | 64.197 | 18.690 | 3.784 | 1.00 | 72.09 | 7 |
| 15 | ATOM | 553 | CA | SER | A | 67 | 65.292 | 19.403 | 4.435 | 1.00 | 72.65 | 6 |
| | ATOM | 554 | CB | SER | A | 67 | 65.063 | 19.425 | 5.943 | 1.00 | 72.61 | 6 |
| | ATOM | 555 | OG | SER | A | 67 | 64.969 | 18.105 | 6.449 | 1.00 | 70.09 | 8 |
| | ATOM | 556 | C | SER | A | 67 | 66.655 | 18.794 | 4.177 | 1.00 | 73.27 | 6 |
| | ATOM | 557 | O | SER | A | 67 | 67.576 | 19.031 | 4.961 | 1.00 | 72.43 | 8 |
| 20 | ATOM | 558 | N | SER | A | 68 | 66.799 | 18.026 | 3.097 | 1.00 | 74.60 | 7 |
| | ATOM | 559 | CA | SER | A | 68 | 68.082 | 17.370 | 2.825 | 1.00 | 76.38 | 6 |
| | ATOM | 560 | CB | SER | A | 68 | 68.006 | 16.490 | 1.564 | 1.00 | 75.57 | 6 |
| | ATOM | 561 | OG | SER | A | 68 | 67.870 | 17.265 | 0.386 | 1.00 | 75.20 | 8 |
| | ATOM | 562 | C | SER | A | 68 | 69.222 | 18.380 | 2.707 | 1.00 | 77.15 | 6 |
| 25 | ATOM | 563 | O | SER | A | 68 | 70.288 | 18.201 | 3.300 | 1.00 | 77.04 | 8 |
| | ATOM | 564 | N | HIS | A | 69 | 68.992 | 19.451 | 1.962 | 1.00 | 78.21 | 7 |
| | ATOM | 565 | CA | HIS | A | 69 | 70.015 | 20.479 | 1.804 | 1.00 | 79.62 | 6 |
| | ATOM | 566 | CB | HIS | A | 69 | 70.445 | 20.578 | 0.341 | 1.00 | 84.04 | 6 |
| | ATOM | 567 | CG | HIS | A | 69 | 71.007 | 19.302 | -0.196 | 1.00 | 88.01 | 6 |
| 30 | ATOM | 568 | CD2 | HIS | A | 69 | 72.208 | 19.022 | -0.759 | 1.00 | 89.20 | 6 |
| | ATOM | 569 | ND1 | HIS | A | 69 | 70.332 | 18.100 | -0.110 | 1.00 | 89.31 | 7 |
| | ATOM | 570 | CE1 | HIS | A | 69 | 71.096 | 17.133 | -0.589 | 1.00 | 90.18 | 6 |
| | ATOM | 571 | NE2 | HIS | A | 69 | 72.240 | 17.666 | -0.988 | 1.00 | 90.99 | 7 |
| | ATOM | 572 | C | HIS | A | 69 | 69.441 | 21.799 | 2.279 | 1.00 | 77.78 | 6 |
| 35 | ATOM | 573 | O | HIS | A | 69 | 69.473 | 22.803 | 1.561 | 1.00 | 77.92 | 8 |
| | ATOM | 574 | N | SER | A | 70 | 68.896 | 21.766 | 3.496 | 1.00 | 75.27 | 7 |
| | ATOM | 575 | CA | SER | A | 70 | 68.300 | 22.931 | 4.141 | 1.00 | 72.21 | 6 |
| | ATOM | 576 | CB | SER | A | 70 | 67.013 | 23.316 | 3.421 | 1.00 | 72.74 | 6 |
| | ATOM | 577 | OG | SER | A | 70 | 66.368 | 22.158 | 2.919 | 1.00 | 74.05 | 8 |
| 40 | ATOM | 578 | C | SER | A | 70 | 68.031 | 22.563 | 5.595 | 1.00 | 69.35 | 6 |
| | ATOM | 579 | O | SER | A | 70 | 68.138 | 21.384 | 5.962 | 1.00 | 70.38 | 8 |
| | ATOM | 580 | N | PRO | A | 71 | 67.710 | 23.563 | 6.450 | 1.00 | 66.44 | 7 |
| | ATOM | 581 | CD | PRO | A | 71 | 67.819 | 24.998 | 6.134 | 1.00 | 64.03 | 6 |
| | ATOM | 582 | CA | PRO | A | 71 | 67.422 | 23.385 | 7.883 | 1.00 | 64.80 | 6 |
| 45 | ATOM | 583 | CB | PRO | A | 71 | 67.106 | 24.805 | 8.334 | 1.00 | 63.49 | 6 |
| | ATOM | 584 | CG | PRO | A | 71 | 68.031 | 25.608 | 7.498 | 1.00 | 61.83 | 6 |
| | ATOM | 585 | C | PRO | A | 71 | 66.295 | 22.395 | 8.223 | 1.00 | 63.99 | 6 |
| | ATOM | 586 | O | PRO | A | 71 | 65.314 | 22.289 | 7.496 | 1.00 | 63.63 | 8 |
| | ATOM | 587 | N | ASP | A | 72 | 66.434 | 21.679 | 9.333 | 1.00 | 63.39 | 7 |
| 50 | ATOM | 588 | CA | ASP | A | 72 | 65.424 | 20.701 | 9.734 | 1.00 | 63.43 | 6 |
| | ATOM | 589 | CB | ASP | A | 72 | 66.056 | 19.634 | 10.617 | 1.00 | 65.69 | 6 |
| | ATOM | 590 | CG | ASP | A | 72 | 67.229 | 18.974 | 9.959 | 1.00 | 70.53 | 6 |
| | ATOM | 591 | OD1 | ASP | A | 72 | 66.985 | 18.216 | 8.988 | 1.00 | 73.68 | 8 |
| | ATOM | 592 | OD2 | ASP | A | 72 | 68.389 | 19.218 | 10.390 | 1.00 | 71.00 | 8 |
| 55 | ATOM | 593 | C | ASP | A | 72 | 64.307 | 21.356 | 10.520 | 1.00 | 62.20 | 6 |
| | ATOM | 594 | O | ASP | A | 72 | 63.164 | 20.878 | 10.520 | 1.00 | 61.88 | 8 |
| | ATOM | 595 | N | GLN | A | 73 | 64.653 | 22.457 | 11.175 | 1.00 | 59.83 | 7 |
| | ATOM | 596 | CA | GLN | A | 73 | 63.738 | 23.186 | 12.041 | 1.00 | 59.45 | 6 |
| | ATOM | 597 | CB | GLN | A | 73 | 64.083 | 22.901 | 13.489 | 1.00 | 60.33 | 6 |
| 60 | ATOM | 598 | CG | GLN | A | 73 | 63.720 | 21.569 | 14.035 | 1.00 | 63.59 | 6 |
| | ATOM | 599 | CD | GLN | A | 73 | 64.224 | 21.462 | 15.459 | 1.00 | 68.15 | 6 |

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|----|------|-----|-----|----------|--------|--------|--------|------|---------|
| 5 | ATOM | 600 | OE1 | GLN A 73 | 65.425 | 21.595 | 15.699 | 1.00 | 70.61 8 |
| | ATOM | 601 | NE2 | GLN A 73 | 63.316 | 21.249 | 16.416 | 1.00 | 69.73 7 |
| | ATOM | 602 | C | GLN A 73 | 63.779 | 24.703 | 11.886 | 1.00 | 57.04 6 |
| | ATOM | 603 | O | GLN A 73 | 64.798 | 25.280 | 11.490 | 1.00 | 58.19 8 |
| | ATOM | 604 | N | VAL A 74 | 62.670 | 25.336 | 12.243 | 1.00 | 52.68 7 |
| 10 | ATOM | 605 | CA | VAL A 74 | 62.557 | 26.782 | 12.211 | 1.00 | 50.24 6 |
| | ATOM | 606 | CB | VAL A 74 | 62.036 | 27.279 | 10.859 | 1.00 | 48.70 6 |
| | ATOM | 607 | CG1 | VAL A 74 | 63.066 | 27.034 | 9.794 | 1.00 | 49.74 6 |
| | ATOM | 608 | CG2 | VAL A 74 | 60.738 | 26.584 | 10.515 | 1.00 | 47.98 6 |
| | ATOM | 609 | C | VAL A 74 | 61.580 | 27.201 | 13.310 | 1.00 | 49.74 6 |
| 15 | ATOM | 610 | O | VAL A 74 | 60.756 | 26.401 | 13.754 | 1.00 | 48.96 8 |
| | ATOM | 611 | N | SER A 75 | 61.691 | 28.442 | 13.769 | 1.00 | 47.62 7 |
| | ATOM | 612 | CA | SER A 75 | 60.792 | 28.954 | 14.787 | 1.00 | 44.06 6 |
| | ATOM | 613 | CB | SER A 75 | 61.525 | 29.902 | 15.728 | 1.00 | 44.67 6 |
| | ATOM | 614 | OG | SER A 75 | 62.241 | 29.188 | 16.710 | 1.00 | 46.37 8 |
| 20 | ATOM | 615 | C | SER A 75 | 59.668 | 29.688 | 14.084 | 1.00 | 43.07 6 |
| | ATOM | 616 | O | SER A 75 | 59.894 | 30.657 | 13.358 | 1.00 | 42.11 8 |
| | ATOM | 617 | N | VAL A 76 | 58.451 | 29.214 | 14.307 | 1.00 | 42.71 7 |
| | ATOM | 618 | CA | VAL A 76 | 57.272 | 29.792 | 13.687 | 1.00 | 43.33 6 |
| | ATOM | 619 | CB | VAL A 76 | 56.482 | 28.711 | 12.936 | 1.00 | 44.34 6 |
| 25 | ATOM | 620 | CG1 | VAL A 76 | 55.247 | 29.315 | 12.298 | 1.00 | 44.97 6 |
| | ATOM | 621 | CG2 | VAL A 76 | 57.359 | 28.058 | 11.894 | 1.00 | 43.12 6 |
| | ATOM | 622 | C | VAL A 76 | 56.335 | 30.436 | 14.704 | 1.00 | 44.16 6 |
| | ATOM | 623 | O | VAL A 76 | 56.093 | 29.882 | 15.773 | 1.00 | 45.89 8 |
| | ATOM | 624 | N | PRO A 77 | 55.798 | 31.624 | 14.388 | 1.00 | 43.19 7 |
| 30 | ATOM | 625 | CD | PRO A 77 | 56.162 | 32.556 | 13.311 | 1.00 | 41.24 6 |
| | ATOM | 626 | CA | PRO A 77 | 54.884 | 32.266 | 15.334 | 1.00 | 41.49 6 |
| | ATOM | 627 | CB | PRO A 77 | 54.619 | 33.615 | 14.691 | 1.00 | 41.13 6 |
| | ATOM | 628 | CG | PRO A 77 | 55.886 | 33.884 | 13.950 | 1.00 | 41.89 6 |
| | ATOM | 629 | C | PRO A 77 | 53.617 | 31.439 | 15.453 | 1.00 | 40.82 6 |
| 35 | ATOM | 630 | O | PRO A 77 | 53.112 | 30.919 | 14.471 | 1.00 | 39.55 8 |
| | ATOM | 631 | N | ILE A 78 | 53.116 | 31.318 | 16.671 | 1.00 | 42.42 7 |
| | ATOM | 632 | CA | ILE A 78 | 51.908 | 30.556 | 16.959 | 1.00 | 42.14 6 |
| | ATOM | 633 | CB | ILE A 78 | 51.526 | 30.751 | 18.441 | 1.00 | 42.09 6 |
| | ATOM | 634 | CG2 | ILE A 78 | 50.105 | 30.357 | 18.712 | 1.00 | 43.53 6 |
| 40 | ATOM | 635 | CG1 | ILE A 78 | 52.464 | 29.921 | 19.285 | 1.00 | 43.22 6 |
| | ATOM | 636 | CD1 | ILE A 78 | 52.585 | 28.513 | 18.784 | 1.00 | 43.92 6 |
| | ATOM | 637 | C | ILE A 78 | 50.749 | 30.942 | 16.057 | 1.00 | 43.58 6 |
| | ATOM | 638 | O | ILE A 78 | 49.985 | 30.096 | 15.624 | 1.00 | 45.64 8 |
| | ATOM | 639 | N | SER A 79 | 50.642 | 32.229 | 15.768 | 1.00 | 43.79 7 |
| 45 | ATOM | 640 | CA | SER A 79 | 49.588 | 32.767 | 14.918 | 1.00 | 44.38 6 |
| | ATOM | 641 | CB | SER A 79 | 49.666 | 34.292 | 14.934 | 1.00 | 44.81 6 |
| | ATOM | 642 | OG | SER A 79 | 50.972 | 34.732 | 14.584 | 1.00 | 45.88 8 |
| | ATOM | 643 | C | SER A 79 | 49.590 | 32.295 | 13.465 | 1.00 | 43.50 6 |
| | ATOM | 644 | O | SER A 79 | 48.607 | 32.498 | 12.758 | 1.00 | 42.80 8 |
| 50 | ATOM | 645 | N | SER A 80 | 50.685 | 31.683 | 13.016 | 1.00 | 42.62 7 |
| | ATOM | 646 | CA | SER A 80 | 50.774 | 31.216 | 11.639 | 1.00 | 42.84 6 |
| | ATOM | 647 | CB | SER A 80 | 52.137 | 31.555 | 11.043 | 1.00 | 44.68 6 |
| | ATOM | 648 | OG | SER A 80 | 52.308 | 32.956 | 10.932 | 1.00 | 51.59 8 |
| | ATOM | 649 | C | SER A 80 | 50.534 | 29.726 | 11.502 | 1.00 | 44.69 6 |
| 55 | ATOM | 650 | O | SER A 80 | 50.596 | 29.184 | 10.402 | 1.00 | 43.97 8 |
| | ATOM | 651 | N | LEU A 81 | 50.248 | 29.068 | 12.620 | 1.00 | 45.13 7 |
| | ATOM | 652 | CA | LEU A 81 | 50.003 | 27.631 | 12.631 | 1.00 | 41.19 6 |
| | ATOM | 653 | CB | LEU A 81 | 51.061 | 26.926 | 13.467 | 1.00 | 39.92 6 |
| | ATOM | 654 | CG | LEU A 81 | 52.534 | 27.167 | 13.185 | 1.00 | 41.52 6 |
| 60 | ATOM | 655 | CD1 | LEU A 81 | 53.356 | 26.677 | 14.355 | 1.00 | 39.70 6 |
| | ATOM | 656 | CD2 | LEU A 81 | 52.922 | 26.464 | 11.918 | 1.00 | 42.52 6 |
| | ATOM | 657 | C | LEU A 81 | 48.672 | 27.340 | 13.272 | 1.00 | 39.47 6 |
| | ATOM | 658 | O | LEU A 81 | 48.089 | 28.197 | 13.921 | 1.00 | 40.21 8 |
| | ATOM | 659 | N | TRP A 82 | 48.191 | 26.122 | 13.081 | 1.00 | 38.46 7 |
| | ATOM | 660 | CA | TRP A 82 | 46.965 | 25.694 | 13.720 | 1.00 | 37.32 6 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 661 | CB | TRP | A | 82 | 46.346 | 24.494 | 13.006 | 1.00 | 36.83 | 6 |
| | ATOM | 662 | CG | TRP | A | 82 | 45.274 | 23.818 | 13.829 | 1.00 | 40.60 | 6 |
| | ATOM | 663 | CD2 | TRP | A | 82 | 45.459 | 22.741 | 14.757 | 1.00 | 39.63 | 6 |
| | ATOM | 664 | CE2 | TRP | A | 82 | 44.213 | 22.499 | 15.369 | 1.00 | 38.33 | 6 |
| | ATOM | 665 | CE3 | TRP | A | 82 | 46.560 | 21.961 | 15.132 | 1.00 | 40.54 | 6 |
| 10 | ATOM | 666 | CD1 | TRP | A | 82 | 43.948 | 24.170 | 13.914 | 1.00 | 39.43 | 6 |
| | ATOM | 667 | NE1 | TRP | A | 82 | 43.311 | 23.383 | 14.839 | 1.00 | 39.00 | 7 |
| | ATOM | 668 | CZ2 | TRP | A | 82 | 44.040 | 21.511 | 16.332 | 1.00 | 38.94 | 6 |
| | ATOM | 669 | CZ3 | TRP | A | 82 | 46.388 | 20.982 | 16.088 | 1.00 | 39.99 | 6 |
| | ATOM | 670 | CH2 | TRP | A | 82 | 45.135 | 20.764 | 16.678 | 1.00 | 39.88 | 6 |
| 15 | ATOM | 671 | C | TRP | A | 82 | 47.485 | 25.241 | 15.064 | 1.00 | 36.99 | 6 |
| | ATOM | 672 | O | TRP | A | 82 | 48.559 | 24.661 | 15.142 | 1.00 | 38.93 | 8 |
| | ATOM | 673 | N | VAL | A | 83 | 46.744 | 25.503 | 16.123 | 1.00 | 37.43 | 7 |
| | ATOM | 674 | CA | VAL | A | 83 | 47.179 | 25.086 | 17.437 | 1.00 | 37.48 | 6 |
| | ATOM | 675 | CB | VAL | A | 83 | 47.729 | 26.300 | 18.209 | 1.00 | 37.40 | 6 |
| 20 | ATOM | 676 | CG1 | VAL | A | 83 | 47.901 | 25.984 | 19.655 | 1.00 | 43.51 | 6 |
| | ATOM | 677 | CG2 | VAL | A | 83 | 49.054 | 26.688 | 17.644 | 1.00 | 37.34 | 6 |
| | ATOM | 678 | C | VAL | A | 83 | 46.011 | 24.437 | 18.175 | 1.00 | 39.74 | 6 |
| | ATOM | 679 | O | VAL | A | 83 | 44.858 | 24.823 | 17.997 | 1.00 | 42.50 | 8 |
| | ATOM | 680 | N | PRO | A | 84 | 46.290 | 23.408 | 18.982 | 1.00 | 39.54 | 7 |
| 25 | ATOM | 681 | CD | PRO | A | 84 | 47.594 | 22.745 | 19.134 | 1.00 | 41.22 | 6 |
| | ATOM | 682 | CA | PRO | A | 84 | 45.263 | 22.701 | 19.752 | 1.00 | 38.54 | 6 |
| | ATOM | 683 | CB | PRO | A | 84 | 46.079 | 21.690 | 20.558 | 1.00 | 39.94 | 6 |
| | ATOM | 684 | CG | PRO | A | 84 | 47.202 | 21.381 | 19.663 | 1.00 | 41.42 | 6 |
| | ATOM | 685 | C | PRO | A | 84 | 44.509 | 23.663 | 20.658 | 1.00 | 36.09 | 6 |
| 30 | ATOM | 686 | O | PRO | A | 84 | 45.121 | 24.469 | 21.342 | 1.00 | 35.57 | 8 |
| | ATOM | 687 | N | ASP | A | 85 | 43.186 | 23.576 | 20.668 | 1.00 | 32.88 | 7 |
| | ATOM | 688 | CA | ASP | A | 85 | 42.397 | 24.458 | 21.505 | 1.00 | 34.36 | 6 |
| | ATOM | 689 | CB | ASP | A | 85 | 41.014 | 24.668 | 20.898 | 1.00 | 35.14 | 6 |
| | ATOM | 690 | CG | ASP | A | 85 | 40.268 | 23.381 | 20.696 | 1.00 | 37.78 | 6 |
| 35 | ATOM | 691 | OD1 | ASP | A | 85 | 40.897 | 22.388 | 20.290 | 1.00 | 40.24 | 8 |
| | ATOM | 692 | OD2 | ASP | A | 85 | 39.050 | 23.367 | 20.927 | 1.00 | 37.65 | 8 |
| | ATOM | 693 | C | ASP | A | 85 | 42.277 | 23.906 | 22.910 | 1.00 | 35.33 | 6 |
| | ATOM | 694 | O | ASP | A | 85 | 41.180 | 23.726 | 23.420 | 1.00 | 38.82 | 8 |
| | ATOM | 695 | N | LEU | A | 86 | 43.418 | 23.644 | 23.528 | 1.00 | 32.24 | 7 |
| 40 | ATOM | 696 | CA | LEU | A | 86 | 43.459 | 23.106 | 24.869 | 1.00 | 35.18 | 6 |
| | ATOM | 697 | CB | LEU | A | 86 | 44.878 | 22.670 | 25.208 | 1.00 | 34.63 | 6 |
| | ATOM | 698 | CG | LEU | A | 86 | 45.435 | 21.585 | 24.311 | 1.00 | 35.36 | 6 |
| | ATOM | 699 | CD1 | LEU | A | 86 | 46.842 | 21.241 | 24.749 | 1.00 | 34.84 | 6 |
| | ATOM | 700 | CD2 | LEU | A | 86 | 44.530 | 20.376 | 24.386 | 1.00 | 35.68 | 6 |
| 45 | ATOM | 701 | C | LEU | A | 86 | 42.973 | 24.086 | 25.925 | 1.00 | 36.01 | 6 |
| | ATOM | 702 | O | LEU | A | 86 | 43.141 | 25.283 | 25.800 | 1.00 | 37.75 | 8 |
| | ATOM | 703 | N | ALA | A | 87 | 42.378 | 23.556 | 26.979 | 1.00 | 38.03 | 7 |
| | ATOM | 704 | CA | ALA | A | 87 | 41.870 | 24.369 | 28.060 | 1.00 | 38.29 | 6 |
| | ATOM | 705 | CB | ALA | A | 87 | 40.428 | 24.674 | 27.811 | 1.00 | 36.17 | 6 |
| 50 | ATOM | 706 | C | ALA | A | 87 | 42.022 | 23.605 | 29.371 | 1.00 | 41.08 | 6 |
| | ATOM | 707 | O | ALA | A | 87 | 41.798 | 22.399 | 29.407 | 1.00 | 43.90 | 8 |
| | ATOM | 708 | N | ALA | A | 88 | 42.431 | 24.290 | 30.436 | 1.00 | 39.68 | 7 |
| | ATOM | 709 | CA | ALA | A | 88 | 42.558 | 23.639 | 31.726 | 1.00 | 38.37 | 6 |
| | ATOM | 710 | CB | ALA | A | 88 | 43.586 | 24.337 | 32.571 | 1.00 | 34.88 | 6 |
| 55 | ATOM | 711 | C | ALA | A | 88 | 41.180 | 23.729 | 32.376 | 1.00 | 40.65 | 6 |
| | ATOM | 712 | O | ALA | A | 88 | 40.778 | 24.780 | 32.847 | 1.00 | 40.29 | 8 |
| | ATOM | 713 | N | TYR | A | 89 | 40.460 | 22.613 | 32.371 | 1.00 | 42.49 | 7 |
| | ATOM | 714 | CA | TYR | A | 89 | 39.116 | 22.502 | 32.934 | 1.00 | 44.24 | 6 |
| | ATOM | 715 | CB | TYR | A | 89 | 38.727 | 21.023 | 33.052 | 1.00 | 46.70 | 6 |
| 60 | ATOM | 716 | CG | TYR | A | 89 | 38.641 | 20.286 | 31.725 | 1.00 | 51.62 | 6 |
| | ATOM | 717 | CD1 | TYR | A | 89 | 38.462 | 18.902 | 31.684 | 1.00 | 54.35 | 6 |
| | ATOM | 718 | CE1 | TYR | A | 89 | 38.353 | 18.222 | 30.466 | 1.00 | 56.33 | 6 |
| | ATOM | 719 | CD2 | TYR | A | 89 | 38.711 | 20.968 | 30.511 | 1.00 | 51.86 | 6 |
| | ATOM | 720 | CE2 | TYR | A | 89 | 38.604 | 20.297 | 29.302 | 1.00 | 53.71 | 6 |
| | ATOM | 721 | CZ | TYR | A | 89 | 38.424 | 18.927 | 29.286 | 1.00 | 55.54 | 6 |

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 722 | OH | TYR | A | 89 | 38.296 | 18.257 | 28.093 | 1.00 | 59.35 | 8 |
| | ATOM | 723 | C | TYR | A | 89 | 38.888 | 23.185 | 34.280 | 1.00 | 43.81 | 6 |
| | ATOM | 724 | O | TYR | A | 89 | 37.808 | 23.735 | 34.518 | 1.00 | 41.70 | 8 |
| | ATOM | 725 | N | ASN | A | 90 | 39.880 | 23.149 | 35.167 | 1.00 | 43.90 | 7 |
| 5 | ATOM | 726 | CA | ASN | A | 90 | 39.709 | 23.781 | 36.473 | 1.00 | 43.12 | 6 |
| | ATOM | 727 | CB | ASN | A | 90 | 39.976 | 22.770 | 37.598 | 1.00 | 40.92 | 6 |
| | ATOM | 728 | CG | ASN | A | 90 | 41.340 | 22.156 | 37.517 | 1.00 | 42.04 | 6 |
| | ATOM | 729 | OD1 | ASN | A | 90 | 41.770 | 21.721 | 36.456 | 1.00 | 43.62 | 8 |
| | ATOM | 730 | ND2 | ASN | A | 90 | 42.033 | 22.102 | 38.646 | 1.00 | 43.25 | 7 |
| 10 | ATOM | 731 | C | ASN | A | 90 | 40.550 | 25.042 | 36.655 | 1.00 | 44.35 | 6 |
| | ATOM | 732 | O | ASN | A | 90 | 40.881 | 25.434 | 37.769 | 1.00 | 46.42 | 8 |
| | ATOM | 733 | N | ALA | A | 91 | 40.902 | 25.673 | 35.543 | 1.00 | 45.44 | 7 |
| | ATOM | 734 | CA | ALA | A | 91 | 41.660 | 26.912 | 35.591 | 1.00 | 45.36 | 6 |
| | ATOM | 735 | CB | ALA | A | 91 | 42.130 | 27.308 | 34.206 | 1.00 | 44.43 | 6 |
| 15 | ATOM | 736 | C | ALA | A | 91 | 40.680 | 27.940 | 36.136 | 1.00 | 45.00 | 6 |
| | ATOM | 737 | O | ALA | A | 91 | 39.522 | 28.000 | 35.729 | 1.00 | 43.71 | 8 |
| | ATOM | 738 | N | ILE | A | 92 | 41.164 | 28.750 | 37.064 | 1.00 | 46.47 | 7 |
| | ATOM | 739 | CA | ILE | A | 92 | 40.359 | 29.753 | 37.734 | 1.00 | 46.18 | 6 |
| | ATOM | 740 | CB | ILE | A | 92 | 40.674 | 29.673 | 39.232 | 1.00 | 47.56 | 6 |
| 20 | ATOM | 741 | CG2 | ILE | A | 92 | 41.595 | 30.797 | 39.634 | 1.00 | 50.92 | 6 |
| | ATOM | 742 | CG1 | ILE | A | 92 | 39.409 | 29.713 | 40.055 | 1.00 | 50.52 | 6 |
| | ATOM | 743 | CD1 | ILE | A | 92 | 39.711 | 29.795 | 41.547 | 1.00 | 51.82 | 6 |
| | ATOM | 744 | C | ILE | A | 92 | 40.659 | 31.157 | 37.177 | 1.00 | 45.80 | 6 |
| | ATOM | 745 | O | ILE | A | 92 | 39.996 | 32.134 | 37.518 | 1.00 | 45.79 | 8 |
| 25 | ATOM | 746 | N | SER | A | 93 | 41.666 | 31.237 | 36.317 | 1.00 | 44.40 | 7 |
| | ATOM | 747 | CA | SER | A | 93 | 42.076 | 32.483 | 35.687 | 1.00 | 41.89 | 6 |
| | ATOM | 748 | CB | SER | A | 93 | 43.248 | 33.080 | 36.445 | 1.00 | 40.83 | 6 |
| | ATOM | 749 | OG | SER | A | 93 | 44.400 | 32.275 | 36.274 | 1.00 | 37.97 | 8 |
| | ATOM | 750 | C | SER | A | 93 | 42.541 | 32.112 | 34.295 | 1.00 | 42.18 | 6 |
| 30 | ATOM | 751 | O | SER | A | 93 | 42.762 | 30.942 | 34.023 | 1.00 | 41.06 | 8 |
| | ATOM | 752 | N | LYS | A | 94 | 42.693 | 33.081 | 33.401 | 1.00 | 43.27 | 7 |
| | ATOM | 753 | CA | LYS | A | 94 | 43.178 | 32.712 | 32.077 | 1.00 | 45.47 | 6 |
| | ATOM | 754 | CB | LYS | A | 94 | 42.703 | 33.680 | 30.988 | 1.00 | 44.26 | 6 |
| | ATOM | 755 | CG | LYS | A | 94 | 42.747 | 35.142 | 31.314 | 1.00 | 44.49 | 6 |
| 35 | ATOM | 756 | CD | LYS | A | 94 | 41.907 | 35.918 | 30.309 | 1.00 | 46.66 | 6 |
| | ATOM | 757 | CE | LYS | A | 94 | 42.209 | 35.470 | 28.885 | 1.00 | 47.75 | 6 |
| | ATOM | 758 | NZ | LYS | A | 94 | 41.443 | 36.237 | 27.873 | 1.00 | 49.19 | 7 |
| | ATOM | 759 | C | LYS | A | 94 | 44.688 | 32.592 | 32.089 | 1.00 | 43.67 | 6 |
| | ATOM | 760 | O | LYS | A | 94 | 45.359 | 33.102 | 32.980 | 1.00 | 44.46 | 8 |
| 40 | ATOM | 761 | N | PRO | A | 95 | 45.243 | 31.889 | 31.105 | 1.00 | 43.23 | 7 |
| | ATOM | 762 | CD | PRO | A | 95 | 44.559 | 31.199 | 30.004 | 1.00 | 41.03 | 6 |
| | ATOM | 763 | CA | PRO | A | 95 | 46.692 | 31.695 | 31.024 | 1.00 | 42.80 | 6 |
| | ATOM | 764 | CB | PRO | A | 95 | 46.858 | 30.719 | 29.862 | 1.00 | 43.77 | 6 |
| | ATOM | 765 | CG | PRO | A | 95 | 45.515 | 30.078 | 29.725 | 1.00 | 43.00 | 6 |
| 45 | ATOM | 766 | C | PRO | A | 95 | 47.480 | 32.962 | 30.783 | 1.00 | 41.84 | 6 |
| | ATOM | 767 | O | PRO | A | 95 | 47.178 | 33.729 | 29.861 | 1.00 | 41.82 | 8 |
| | ATOM | 768 | N | GLU | A | 96 | 48.483 | 33.183 | 31.627 | 1.00 | 40.74 | 7 |
| | ATOM | 769 | CA | GLU | A | 96 | 49.350 | 34.322 | 31.472 | 1.00 | 39.25 | 6 |
| | ATOM | 770 | CB | GLU | A | 96 | 49.704 | 34.960 | 32.817 | 1.00 | 41.50 | 6 |
| 50 | ATOM | 771 | CG | GLU | A | 96 | 50.548 | 36.235 | 32.682 | 1.00 | 46.46 | 6 |
| | ATOM | 772 | CD | GLU | A | 96 | 50.864 | 36.910 | 34.014 | 1.00 | 51.10 | 6 |
| | ATOM | 773 | OE1 | GLU | A | 96 | 50.172 | 36.591 | 35.002 | 1.00 | 55.39 | 8 |
| | ATOM | 774 | OE2 | GLU | A | 96 | 51.784 | 37.772 | 34.079 | 1.00 | 51.01 | 8 |
| | ATOM | 775 | C | GLU | A | 96 | 50.583 | 33.713 | 30.851 | 1.00 | 38.30 | 6 |
| 55 | ATOM | 776 | O | GLU | A | 96 | 51.424 | 33.169 | 31.548 | 1.00 | 37.33 | 8 |
| | ATOM | 777 | N | VAL | A | 97 | 50.662 | 33.770 | 29.528 | 1.00 | 36.80 | 7 |
| | ATOM | 778 | CA | VAL | A | 97 | 51.813 | 33.231 | 28.821 | 1.00 | 37.13 | 6 |
| | ATOM | 779 | CB | VAL | A | 97 | 51.514 | 33.092 | 27.313 | 1.00 | 35.99 | 6 |
| | ATOM | 780 | CG1 | VAL | A | 97 | 52.704 | 32.480 | 26.600 | 1.00 | 34.96 | 6 |
| 60 | ATOM | 781 | CG2 | VAL | A | 97 | 50.287 | 32.222 | 27.122 | 1.00 | 30.36 | 6 |
| | ATOM | 782 | C | VAL | A | 97 | 53.002 | 34.160 | 29.061 | 1.00 | 37.37 | 6 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|---------|
| 5 | ATOM | 783 | O | VAL A 97 | 52.998 | 35.329 | 28.670 | 1.00 | 35.14 8 |
| | ATOM | 784 | N | LEU A 98 | 54.022 | 33.619 | 29.715 | 1.00 | 37.54 7 |
| | ATOM | 785 | CA | LEU A 98 | 55.203 | 34.389 | 30.070 | 1.00 | 39.37 6 |
| | ATOM | 786 | CB | LEU A 98 | 55.773 | 33.851 | 31.374 | 1.00 | 38.96 6 |
| | ATOM | 787 | CG | LEU A 98 | 54.848 | 33.662 | 32.568 | 1.00 | 39.17 6 |
| | ATOM | 788 | CD1 | LEU A 98 | 55.522 | 32.772 | 33.576 | 1.00 | 37.89 6 |
| | ATOM | 789 | CD2 | LEU A 98 | 54.501 | 34.997 | 33.169 | 1.00 | 38.95 6 |
| | ATOM | 790 | C | LEU A 98 | 56.317 | 34.387 | 29.033 | 1.00 | 41.78 6 |
| 10 | ATOM | 791 | O | LEU A 98 | 57.310 | 35.114 | 29.177 | 1.00 | 42.77 8 |
| | ATOM | 792 | N | THR A 99 | 56.162 | 33.579 | 27.992 | 1.00 | 39.65 7 |
| | ATOM | 793 | CA | THR A 99 | 57.199 | 33.471 | 26.981 | 1.00 | 37.85 6 |
| | ATOM | 794 | CB | THR A 99 | 57.793 | 32.063 | 27.004 | 1.00 | 39.36 6 |
| | ATOM | 795 | OG1 | THR A 99 | 56.745 | 31.102 | 26.822 | 1.00 | 40.29 8 |
| 15 | ATOM | 796 | CG2 | THR A 99 | 58.490 | 31.812 | 28.325 | 1.00 | 36.68 6 |
| | ATOM | 797 | C | THR A 99 | 56.762 | 33.784 | 25.559 | 1.00 | 37.27 6 |
| | ATOM | 798 | O | THR A 99 | 55.571 | 33.809 | 25.260 | 1.00 | 37.48 8 |
| | ATOM | 799 | N | PRO A 100 | 57.733 | 34.050 | 24.666 | 1.00 | 35.48 7 |
| | ATOM | 800 | CD | PRO A 100 | 59.169 | 34.217 | 24.938 | 1.00 | 34.88 6 |
| 20 | ATOM | 801 | CA | PRO A 100 | 57.450 | 34.356 | 23.268 | 1.00 | 34.86 6 |
| | ATOM | 802 | CB | PRO A 100 | 58.825 | 34.308 | 22.631 | 1.00 | 32.91 6 |
| | ATOM | 803 | CG | PRO A 100 | 59.660 | 34.899 | 23.674 | 1.00 | 33.33 6 |
| | ATOM | 804 | C | PRO A 100 | 56.535 | 33.287 | 22.735 | 1.00 | 34.32 6 |
| | ATOM | 805 | O | PRO A 100 | 56.748 | 32.110 | 22.990 | 1.00 | 37.05 8 |
| 25 | ATOM | 806 | N | GLN A 101 | 55.508 | 33.684 | 22.005 | 1.00 | 35.52 7 |
| | ATOM | 807 | CA | GLN A 101 | 54.591 | 32.698 | 21.483 | 1.00 | 38.08 6 |
| | ATOM | 808 | CB | GLN A 101 | 53.181 | 33.271 | 21.452 | 1.00 | 39.02 6 |
| | ATOM | 809 | CG | GLN A 101 | 52.557 | 33.223 | 22.836 | 1.00 | 42.77 6 |
| | ATOM | 810 | CD | GLN A 101 | 51.356 | 34.102 | 22.965 | 1.00 | 46.68 6 |
| 30 | ATOM | 811 | OE1 | GLN A 101 | 50.383 | 33.943 | 22.239 | 1.00 | 51.63 8 |
| | ATOM | 812 | NE2 | GLN A 101 | 51.408 | 35.045 | 23.900 | 1.00 | 48.84 7 |
| | ATOM | 813 | C | GLN A 101 | 55.006 | 32.145 | 20.144 | 1.00 | 37.60 6 |
| | ATOM | 814 | O | GLN A 101 | 54.331 | 32.329 | 19.136 | 1.00 | 36.16 8 |
| | ATOM | 815 | N | LEU A 102 | 56.138 | 31.445 | 20.177 | 1.00 | 38.73 7 |
| 35 | ATOM | 816 | CA | LEU A 102 | 56.742 | 30.812 | 19.016 | 1.00 | 38.35 6 |
| | ATOM | 817 | CB | LEU A 102 | 58.180 | 31.289 | 18.833 | 1.00 | 36.63 6 |
| | ATOM | 818 | CG | LEU A 102 | 58.411 | 32.792 | 18.709 | 1.00 | 37.99 6 |
| | ATOM | 819 | CD1 | LEU A 102 | 59.890 | 33.054 | 18.550 | 1.00 | 39.54 6 |
| | ATOM | 820 | CD2 | LEU A 102 | 57.650 | 33.343 | 17.538 | 1.00 | 35.40 6 |
| 40 | ATOM | 821 | C | LEU A 102 | 56.763 | 29.311 | 19.200 | 1.00 | 39.23 6 |
| | ATOM | 822 | O | LEU A 102 | 56.933 | 28.809 | 20.302 | 1.00 | 40.34 8 |
| | ATOM | 823 | N | ALA A 103 | 56.574 | 28.595 | 18.104 | 1.00 | 40.83 7 |
| | ATOM | 824 | CA | ALA A 103 | 56.603 | 27.142 | 18.125 | 1.00 | 41.49 6 |
| | ATOM | 825 | CB | ALA A 103 | 55.334 | 26.569 | 17.497 | 1.00 | 41.49 6 |
| 45 | ATOM | 826 | C | ALA A 103 | 57.830 | 26.697 | 17.337 | 1.00 | 42.17 6 |
| | ATOM | 827 | O | ALA A 103 | 58.472 | 27.484 | 16.645 | 1.00 | 43.45 8 |
| | ATOM | 828 | N | ARG A 104 | 58.163 | 25.427 | 17.453 | 1.00 | 43.77 7 |
| | ATOM | 829 | CA | ARG A 104 | 59.309 | 24.893 | 16.750 | 1.00 | 44.63 6 |
| | ATOM | 830 | CB | ARG A 104 | 60.242 | 24.228 | 17.745 | 1.00 | 43.89 6 |
| 50 | ATOM | 831 | CG | ARG A 104 | 61.621 | 23.992 | 17.214 | 1.00 | 45.78 6 |
| | ATOM | 832 | CD | ARG A 104 | 62.362 | 25.277 | 16.950 | 1.00 | 43.65 6 |
| | ATOM | 833 | NE | ARG A 104 | 63.675 | 24.958 | 16.409 | 1.00 | 44.01 7 |
| | ATOM | 834 | CZ | ARG A 104 | 64.618 | 25.848 | 16.124 | 1.00 | 46.53 6 |
| | ATOM | 835 | NH1 | ARG A 104 | 64.411 | 27.147 | 16.327 | 1.00 | 47.99 7 |
| 55 | ATOM | 836 | NH2 | ARG A 104 | 65.775 | 25.432 | 15.632 | 1.00 | 47.13 7 |
| | ATOM | 837 | C | ARG A 104 | 58.770 | 23.878 | 15.754 | 1.00 | 46.81 6 |
| | ATOM | 838 | O | ARG A 104 | 58.042 | 22.961 | 16.124 | 1.00 | 49.12 8 |
| | ATOM | 839 | N | VAL A 105 | 59.097 | 24.049 | 14.482 | 1.00 | 47.69 7 |
| | ATOM | 840 | CA | VAL A 105 | 58.601 | 23.125 | 13.469 | 1.00 | 47.16 6 |
| 60 | ATOM | 841 | CB | VAL A 105 | 57.791 | 23.857 | 12.382 | 1.00 | 44.84 6 |
| | ATOM | 842 | CG1 | VAL A 105 | 57.198 | 22.861 | 11.421 | 1.00 | 41.16 6 |
| | ATOM | 843 | CG2 | VAL A 105 | 56.702 | 24.684 | 13.018 | 1.00 | 45.42 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 844 | C | VAL | A | 105 | 59.731 | 22.355 | 12.799 | 1.00 | 49.71 | 6 |
| | ATOM | 845 | O | VAL | A | 105 | 60.688 | 22.946 | 12.283 | 1.00 | 48.12 | 8 |
| | ATOM | 846 | N | VAL | A | 106 | 59.597 | 21.030 | 12.821 | 1.00 | 50.55 | 7 |
| 5 | ATOM | 847 | CA | VAL | A | 106 | 60.571 | 20.123 | 12.232 | 1.00 | 51.43 | 6 |
| | ATOM | 848 | CB | VAL | A | 106 | 60.648 | 18.816 | 13.037 | 1.00 | 52.44 | 6 |
| | ATOM | 849 | CG1 | VAL | A | 106 | 61.828 | 17.987 | 12.571 | 1.00 | 50.24 | 6 |
| | ATOM | 850 | CG2 | VAL | A | 106 | 60.762 | 19.128 | 14.521 | 1.00 | 52.53 | 6 |
| | ATOM | 851 | C | VAL | A | 106 | 60.142 | 19.809 | 10.805 | 1.00 | 52.38 | 6 |
| 10 | ATOM | 852 | O | VAL | A | 106 | 58.961 | 19.644 | 10.536 | 1.00 | 52.65 | 8 |
| | ATOM | 853 | N | SER | A | 107 | 61.101 | 19.718 | 9.895 | 1.00 | 52.34 | 7 |
| | ATOM | 854 | CA | SER | A | 107 | 60.803 | 19.447 | 8.492 | 1.00 | 54.32 | 6 |
| | ATOM | 855 | CB | SER | A | 107 | 62.111 | 19.185 | 7.735 | 1.00 | 55.62 | 6 |
| | ATOM | 856 | OG | SER | A | 107 | 62.965 | 18.316 | 8.462 | 1.00 | 60.14 | 8 |
| 15 | ATOM | 857 | C | SER | A | 107 | 59.795 | 18.328 | 8.186 | 1.00 | 53.69 | 6 |
| | ATOM | 858 | O | SER | A | 107 | 59.191 | 18.304 | 7.111 | 1.00 | 51.90 | 8 |
| | ATOM | 859 | N | ASP | A | 108 | 59.598 | 17.412 | 9.122 | 1.00 | 54.61 | 7 |
| | ATOM | 860 | CA | ASP | A | 108 | 58.667 | 16.318 | 8.890 | 1.00 | 57.15 | 6 |
| | ATOM | 861 | CB | ASP | A | 108 | 59.164 | 15.046 | 9.580 | 1.00 | 58.72 | 6 |
| 20 | ATOM | 862 | CG | ASP | A | 108 | 59.114 | 15.134 | 11.097 | 1.00 | 61.68 | 6 |
| | ATOM | 863 | OD1 | ASP | A | 108 | 59.391 | 16.221 | 11.642 | 1.00 | 64.28 | 8 |
| | ATOM | 864 | OD2 | ASP | A | 108 | 58.816 | 14.105 | 11.747 | 1.00 | 62.23 | 8 |
| | ATOM | 865 | C | ASP | A | 108 | 57.235 | 16.615 | 9.320 | 1.00 | 58.57 | 6 |
| | ATOM | 866 | O | ASP | A | 108 | 56.379 | 15.725 | 9.301 | 1.00 | 58.30 | 8 |
| 25 | ATOM | 867 | N | GLY | A | 109 | 56.979 | 17.865 | 9.703 | 1.00 | 59.14 | 7 |
| | ATOM | 868 | CA | GLY | A | 109 | 55.649 | 18.271 | 10.116 | 1.00 | 58.25 | 6 |
| | ATOM | 869 | C | GLY | A | 109 | 55.397 | 18.166 | 11.602 | 1.00 | 58.69 | 6 |
| | ATOM | 870 | O | GLY | A | 109 | 54.273 | 18.374 | 12.054 | 1.00 | 59.98 | 8 |
| | ATOM | 871 | N | GLU | A | 110 | 56.423 | 17.821 | 12.369 | 1.00 | 58.71 | 7 |
| 30 | ATOM | 872 | CA | GLU | A | 110 | 56.255 | 17.713 | 13.813 | 1.00 | 58.33 | 6 |
| | ATOM | 873 | CB | GLU | A | 110 | 57.380 | 16.871 | 14.425 | 1.00 | 61.59 | 6 |
| | ATOM | 874 | CG | GLU | A | 110 | 57.062 | 16.242 | 15.797 | 1.00 | 66.10 | 6 |
| | ATOM | 875 | CD | GLU | A | 110 | 55.913 | 15.218 | 15.728 | 1.00 | 70.89 | 6 |
| | ATOM | 876 | OE1 | GLU | A | 110 | 55.634 | 14.710 | 14.600 | 1.00 | 70.53 | 8 |
| | ATOM | 877 | OE2 | GLU | A | 110 | 55.303 | 14.916 | 16.800 | 1.00 | 70.77 | 8 |
| 35 | ATOM | 878 | C | GLU | A | 110 | 56.293 | 19.136 | 14.369 | 1.00 | 56.59 | 6 |
| | ATOM | 879 | O | GLU | A | 110 | 57.114 | 19.955 | 13.941 | 1.00 | 54.81 | 8 |
| | ATOM | 880 | N | VAL | A | 111 | 55.392 | 19.425 | 15.307 | 1.00 | 54.27 | 7 |
| | ATOM | 881 | CA | VAL | A | 111 | 55.310 | 20.745 | 15.912 | 1.00 | 52.01 | 6 |
| 40 | ATOM | 882 | CB | VAL | A | 111 | 53.949 | 21.412 | 15.616 | 1.00 | 50.79 | 6 |
| | ATOM | 883 | CG1 | VAL | A | 111 | 53.902 | 22.795 | 16.242 | 1.00 | 47.90 | 6 |
| | ATOM | 884 | CG2 | VAL | A | 111 | 53.718 | 21.489 | 14.115 | 1.00 | 50.80 | 6 |
| | ATOM | 885 | C | VAL | A | 111 | 55.465 | 20.666 | 17.418 | 1.00 | 51.33 | 6 |
| | ATOM | 886 | O | VAL | A | 111 | 54.833 | 19.830 | 18.057 | 1.00 | 50.54 | 8 |
| 45 | ATOM | 887 | N | LEU | A | 112 | 56.300 | 21.539 | 17.979 | 1.00 | 49.64 | 7 |
| | ATOM | 888 | CA | LEU | A | 112 | 56.501 | 21.569 | 19.418 | 1.00 | 50.36 | 6 |
| | ATOM | 889 | CB | LEU | A | 112 | 57.911 | 21.107 | 19.791 | 1.00 | 54.86 | 6 |
| | ATOM | 890 | CG | LEU | A | 112 | 58.651 | 20.020 | 18.989 | 1.00 | 59.01 | 6 |
| | ATOM | 891 | CD1 | LEU | A | 112 | 57.699 | 18.865 | 18.631 | 1.00 | 60.90 | 6 |
| 50 | ATOM | 892 | CD2 | LEU | A | 112 | 59.248 | 20.632 | 17.727 | 1.00 | 57.28 | 6 |
| | ATOM | 893 | C | LEU | A | 112 | 56.297 | 22.980 | 19.946 | 1.00 | 49.94 | 6 |
| | ATOM | 894 | O | LEU | A | 112 | 57.004 | 23.893 | 19.553 | 1.00 | 49.38 | 8 |
| | ATOM | 895 | N | TYR | A | 113 | 55.323 | 23.151 | 20.833 | 1.00 | 49.46 | 7 |
| | ATOM | 896 | CA | TYR | A | 113 | 55.036 | 24.446 | 21.437 | 1.00 | 47.23 | 6 |
| 55 | ATOM | 897 | CB | TYR | A | 113 | 53.643 | 24.939 | 21.021 | 1.00 | 45.72 | 6 |
| | ATOM | 898 | CG | TYR | A | 113 | 53.222 | 26.279 | 21.621 | 1.00 | 46.02 | 6 |
| | ATOM | 899 | CD1 | TYR | A | 113 | 54.092 | 27.364 | 21.654 | 1.00 | 42.86 | 6 |
| | ATOM | 900 | CE1 | TYR | A | 113 | 53.691 | 28.588 | 22.179 | 1.00 | 43.03 | 6 |
| | ATOM | 901 | CD2 | TYR | A | 113 | 51.936 | 26.462 | 22.131 | 1.00 | 45.25 | 6 |
| 60 | ATOM | 902 | CE2 | TYR | A | 113 | 51.533 | 27.682 | 22.653 | 1.00 | 41.00 | 6 |
| | ATOM | 903 | CZ | TYR | A | 113 | 52.410 | 28.740 | 22.677 | 1.00 | 42.42 | 6 |
| | ATOM | 904 | OH | TYR | A | 113 | 52.008 | 29.952 | 23.211 | 1.00 | 42.79 | 8 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 905 | C | TYR | A | 113 | 55.097 | 24.250 | 22.936 | 1.00 | 47.38 | 6 |
| | ATOM | 906 | O | TYR | A | 113 | 54.304 | 23.508 | 23.506 | 1.00 | 47.08 | 8 |
| | ATOM | 907 | N | MET | A | 114 | 56.047 | 24.916 | 23.577 | 1.00 | 48.38 | 7 |
| | ATOM | 908 | CA | MET | A | 114 | 56.205 | 24.788 | 25.015 | 1.00 | 48.39 | 6 |
| 5 | ATOM | 909 | CB | MET | A | 114 | 57.485 | 24.020 | 25.304 | 1.00 | 52.09 | 6 |
| | ATOM | 910 | CG | MET | A | 114 | 57.675 | 23.679 | 26.739 | 1.00 | 59.10 | 6 |
| | ATOM | 911 | SD | MET | A | 114 | 59.383 | 23.282 | 26.925 | 1.00 | 67.20 | 16 |
| | ATOM | 912 | CE | MET | A | 114 | 59.324 | 21.518 | 26.416 | 1.00 | 67.26 | 6 |
| | ATOM | 913 | C | MET | A | 114 | 56.245 | 26.148 | 25.701 | 1.00 | 46.12 | 6 |
| 10 | ATOM | 914 | O | MET | A | 114 | 57.308 | 26.660 | 26.027 | 1.00 | 46.76 | 8 |
| | ATOM | 915 | N | PRO | A | 115 | 55.076 | 26.754 | 25.922 | 1.00 | 44.80 | 7 |
| | ATOM | 916 | CD | PRO | A | 115 | 53.740 | 26.329 | 25.463 | 1.00 | 44.54 | 6 |
| | ATOM | 917 | CA | PRO | A | 115 | 55.005 | 28.059 | 26.575 | 1.00 | 44.08 | 6 |
| | ATOM | 918 | CB | PRO | A | 115 | 53.675 | 28.598 | 26.075 | 1.00 | 45.01 | 6 |
| 15 | ATOM | 919 | CG | PRO | A | 115 | 52.831 | 27.366 | 26.077 | 1.00 | 43.44 | 6 |
| | ATOM | 920 | C | PRO | A | 115 | 55.030 | 27.935 | 28.102 | 1.00 | 43.24 | 6 |
| | ATOM | 921 | O | PRO | A | 115 | 54.552 | 26.947 | 28.664 | 1.00 | 40.79 | 8 |
| | ATOM | 922 | N | SER | A | 116 | 55.599 | 28.929 | 28.771 | 1.00 | 42.36 | 7 |
| | ATOM | 923 | CA | SER | A | 116 | 55.627 | 28.911 | 30.227 | 1.00 | 42.64 | 6 |
| 20 | ATOM | 924 | CB | SER | A | 116 | 56.851 | 29.624 | 30.764 | 1.00 | 40.99 | 6 |
| | ATOM | 925 | OG | SER | A | 116 | 56.852 | 29.573 | 32.169 | 1.00 | 41.56 | 8 |
| | ATOM | 926 | C | SER | A | 116 | 54.382 | 29.658 | 30.653 | 1.00 | 42.71 | 6 |
| | ATOM | 927 | O | SER | A | 116 | 54.184 | 30.809 | 30.266 | 1.00 | 44.52 | 8 |
| | ATOM | 928 | N | ILE | A | 117 | 53.545 | 29.006 | 31.446 | 1.00 | 41.18 | 7 |
| 25 | ATOM | 929 | CA | ILE | A | 117 | 52.303 | 29.616 | 31.879 | 1.00 | 40.12 | 6 |
| | ATOM | 930 | CB | ILE | A | 117 | 51.104 | 28.814 | 31.325 | 1.00 | 37.67 | 6 |
| | ATOM | 931 | CG2 | ILE | A | 117 | 49.805 | 29.400 | 31.819 | 1.00 | 38.25 | 6 |
| | ATOM | 932 | CG1 | ILE | A | 117 | 51.134 | 28.825 | 29.798 | 1.00 | 36.76 | 6 |
| | ATOM | 933 | CD1 | ILE | A | 117 | 50.212 | 27.822 | 29.169 | 1.00 | 33.48 | 6 |
| 30 | ATOM | 934 | C | ILE | A | 117 | 52.114 | 29.768 | 33.388 | 1.00 | 41.31 | 6 |
| | ATOM | 935 | O | ILE | A | 117 | 52.444 | 28.876 | 34.168 | 1.00 | 43.78 | 8 |
| | ATOM | 936 | N | ARG | A | 118 | 51.607 | 30.925 | 33.795 | 1.00 | 41.35 | 7 |
| | ATOM | 937 | CA | ARG | A | 118 | 51.283 | 31.153 | 35.194 | 1.00 | 41.26 | 6 |
| | ATOM | 938 | CB | ARG | A | 118 | 51.789 | 32.496 | 35.709 | 1.00 | 38.56 | 6 |
| 35 | ATOM | 939 | CG | ARG | A | 118 | 51.290 | 32.758 | 37.113 | 1.00 | 37.29 | 6 |
| | ATOM | 940 | CD | ARG | A | 118 | 52.006 | 33.883 | 37.817 | 1.00 | 38.24 | 6 |
| | ATOM | 941 | NE | ARG | A | 118 | 51.453 | 34.066 | 39.150 | 1.00 | 41.49 | 7 |
| | ATOM | 942 | CZ | ARG | A | 118 | 52.006 | 34.794 | 40.107 | 1.00 | 43.10 | 6 |
| | ATOM | 943 | NH1 | ARG | A | 118 | 53.148 | 35.423 | 39.892 | 1.00 | 46.98 | 7 |
| 40 | ATOM | 944 | NH2 | ARG | A | 118 | 51.417 | 34.890 | 41.282 | 1.00 | 43.21 | 7 |
| | ATOM | 945 | C | ARG | A | 118 | 49.765 | 31.156 | 35.179 | 1.00 | 41.21 | 6 |
| | ATOM | 946 | O | ARG | A | 118 | 49.144 | 31.842 | 34.374 | 1.00 | 41.57 | 8 |
| | ATOM | 947 | N | GLN | A | 119 | 49.152 | 30.394 | 36.063 | 1.00 | 41.94 | 7 |
| | ATOM | 948 | CA | GLN | A | 119 | 47.702 | 30.329 | 36.056 | 1.00 | 43.44 | 6 |
| 45 | ATOM | 949 | CB | GLN | A | 119 | 47.292 | 29.433 | 34.895 | 1.00 | 41.21 | 6 |
| | ATOM | 950 | CG | GLN | A | 119 | 45.825 | 29.257 | 34.672 | 1.00 | 43.47 | 6 |
| | ATOM | 951 | CD | GLN | A | 119 | 45.552 | 28.554 | 33.364 | 1.00 | 41.25 | 6 |
| | ATOM | 952 | OE1 | GLN | A | 119 | 46.333 | 27.721 | 32.931 | 1.00 | 42.28 | 8 |
| | ATOM | 953 | NE2 | GLN | A | 119 | 44.439 | 28.877 | 32.736 | 1.00 | 42.81 | 7 |
| 50 | ATOM | 954 | C | GLN | A | 119 | 47.183 | 29.801 | 37.385 | 1.00 | 44.09 | 6 |
| | ATOM | 955 | O | GLN | A | 119 | 47.866 | 29.041 | 38.062 | 1.00 | 43.59 | 8 |
| | ATOM | 956 | N | ARG | A | 120 | 45.990 | 30.228 | 37.778 | 1.00 | 46.26 | 7 |
| | ATOM | 957 | CA | ARG | A | 120 | 45.433 | 29.762 | 39.036 | 1.00 | 48.60 | 6 |
| | ATOM | 958 | CB | ARG | A | 120 | 44.780 | 30.900 | 39.797 | 1.00 | 51.27 | 6 |
| 55 | ATOM | 959 | CG | ARG | A | 120 | 45.705 | 32.036 | 40.096 | 1.00 | 60.62 | 6 |
| | ATOM | 960 | CD | ARG | A | 120 | 45.261 | 32.728 | 41.362 | 1.00 | 67.20 | 6 |
| | ATOM | 961 | NE | ARG | A | 120 | 45.730 | 32.045 | 42.575 | 1.00 | 69.70 | 7 |
| | ATOM | 962 | CZ | ARG | A | 120 | 44.989 | 31.859 | 43.668 | 1.00 | 69.76 | 6 |
| | ATOM | 963 | NH1 | ARG | A | 120 | 43.728 | 32.279 | 43.709 | 1.00 | 68.36 | 7 |
| 60 | ATOM | 964 | NH2 | ARG | A | 120 | 45.533 | 31.307 | 44.748 | 1.00 | 70.33 | 7 |
| | ATOM | 965 | C | ARG | A | 120 | 44.414 | 28.669 | 38.804 | 1.00 | 48.02 | 6 |

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|----|------|------|---------------|--------|--------|--------|------|-------|----|
| 5 | ATOM | 966 | O ARG A 120 | 43.706 | 28.669 | 37.788 | 1.00 | 46.40 | 8 |
| | ATOM | 967 | N PHE A 121 | 44.341 | 27.739 | 39.753 | 1.00 | 46.74 | 7 |
| | ATOM | 968 | CA PHE A 121 | 43.406 | 26.628 | 39.648 | 1.00 | 48.15 | 6 |
| | ATOM | 969 | CB PHE A 121 | 44.129 | 25.330 | 39.301 | 1.00 | 45.72 | 6 |
| | ATOM | 970 | CG PHE A 121 | 44.973 | 25.415 | 38.074 | 1.00 | 44.95 | 6 |
| 10 | ATOM | 971 | CD1 PHE A 121 | 46.240 | 25.993 | 38.122 | 1.00 | 43.54 | 6 |
| | ATOM | 972 | CD2 PHE A 121 | 44.495 | 24.944 | 36.866 | 1.00 | 41.66 | 6 |
| | ATOM | 973 | CE1 PHE A 121 | 47.011 | 26.099 | 36.986 | 1.00 | 42.05 | 6 |
| | ATOM | 974 | CE2 PHE A 121 | 45.257 | 25.047 | 35.733 | 1.00 | 41.56 | 6 |
| | ATOM | 975 | CZ PHE A 121 | 46.521 | 25.628 | 35.790 | 1.00 | 42.24 | 6 |
| 15 | ATOM | 976 | C PHE A 121 | 42.622 | 26.376 | 40.908 | 1.00 | 49.43 | 6 |
| | ATOM | 977 | O PHE A 121 | 42.996 | 26.810 | 42.001 | 1.00 | 49.47 | 8 |
| | ATOM | 978 | N SER A 122 | 41.524 | 25.653 | 40.727 | 1.00 | 51.17 | 7 |
| | ATOM | 979 | CA SER A 122 | 40.657 | 25.250 | 41.823 | 1.00 | 52.06 | 6 |
| | ATOM | 980 | CB SER A 122 | 39.193 | 25.501 | 41.477 | 1.00 | 52.69 | 6 |
| 20 | ATOM | 981 | OG SER A 122 | 38.354 | 25.046 | 42.520 | 1.00 | 51.12 | 8 |
| | ATOM | 982 | C SER A 122 | 40.896 | 23.754 | 41.978 | 1.00 | 52.70 | 6 |
| | ATOM | 983 | O SER A 122 | 40.529 | 22.966 | 41.103 | 1.00 | 51.13 | 8 |
| | ATOM | 984 | N CYS A 123 | 41.543 | 23.369 | 43.070 | 1.00 | 52.97 | 7 |
| | ATOM | 985 | CA CYS A 123 | 41.820 | 21.967 | 43.312 | 1.00 | 56.03 | 6 |
| 25 | ATOM | 986 | C CYS A 123 | 42.017 | 21.693 | 44.803 | 1.00 | 59.48 | 6 |
| | ATOM | 987 | O CYS A 123 | 41.882 | 22.602 | 45.634 | 1.00 | 60.13 | 8 |
| | ATOM | 988 | CB CYS A 123 | 43.052 | 21.555 | 42.534 | 1.00 | 53.78 | 6 |
| | ATOM | 989 | SG CYS A 123 | 44.483 | 22.558 | 42.968 | 1.00 | 56.89 | 16 |
| | ATOM | 990 | N ASP A 124 | 42.342 | 20.443 | 45.143 | 1.00 | 61.91 | 7 |
| 30 | ATOM | 991 | CA ASP A 124 | 42.525 | 20.084 | 46.542 | 1.00 | 63.81 | 6 |
| | ATOM | 992 | CB ASP A 124 | 42.391 | 18.571 | 46.749 | 1.00 | 65.05 | 6 |
| | ATOM | 993 | CG ASP A 124 | 41.828 | 18.226 | 48.128 | 1.00 | 66.74 | 6 |
| | ATOM | 994 | OD1 ASP A 124 | 42.113 | 18.973 | 49.103 | 1.00 | 65.03 | 8 |
| | ATOM | 995 | OD2 ASP A 124 | 41.101 | 17.209 | 48.234 | 1.00 | 67.39 | 8 |
| 35 | ATOM | 996 | C ASP A 124 | 43.857 | 20.543 | 47.110 | 1.00 | 63.72 | 6 |
| | ATOM | 997 | O ASP A 124 | 44.910 | 20.036 | 46.745 | 1.00 | 64.11 | 8 |
| | ATOM | 998 | N VAL A 125 | 43.794 | 21.495 | 48.031 | 1.00 | 64.49 | 7 |
| | ATOM | 999 | CA VAL A 125 | 44.981 | 22.042 | 48.681 | 1.00 | 63.28 | 6 |
| | ATOM | 1000 | CB VAL A 125 | 44.861 | 23.578 | 48.804 | 1.00 | 62.29 | 6 |
| 40 | ATOM | 1001 | CG1 VAL A 125 | 46.058 | 24.135 | 49.539 | 1.00 | 61.76 | 6 |
| | ATOM | 1002 | CG2 VAL A 125 | 44.735 | 24.194 | 47.429 | 1.00 | 61.51 | 6 |
| | ATOM | 1003 | C VAL A 125 | 45.190 | 21.449 | 50.078 | 1.00 | 63.42 | 6 |
| | ATOM | 1004 | O VAL A 125 | 46.283 | 21.534 | 50.632 | 1.00 | 63.08 | 8 |
| | ATOM | 1005 | N SER A 126 | 44.141 | 20.848 | 50.641 | 1.00 | 64.34 | 7 |
| 45 | ATOM | 1006 | CA SER A 126 | 44.218 | 20.252 | 51.981 | 1.00 | 64.43 | 6 |
| | ATOM | 1007 | CB SER A 126 | 42.924 | 19.503 | 52.302 | 1.00 | 63.15 | 6 |
| | ATOM | 1008 | OG SER A 126 | 42.723 | 18.465 | 51.371 | 1.00 | 58.95 | 8 |
| | ATOM | 1009 | C SER A 126 | 45.414 | 19.306 | 52.128 | 1.00 | 64.40 | 6 |
| | ATOM | 1010 | O SER A 126 | 45.636 | 18.420 | 51.299 | 1.00 | 62.89 | 8 |
| 50 | ATOM | 1011 | N GLY A 127 | 46.188 | 19.510 | 53.186 | 1.00 | 65.00 | 7 |
| | ATOM | 1012 | CA GLY A 127 | 47.343 | 18.676 | 53.416 | 1.00 | 67.55 | 6 |
| | ATOM | 1013 | C GLY A 127 | 48.647 | 19.293 | 52.939 | 1.00 | 71.25 | 6 |
| | ATOM | 1014 | O GLY A 127 | 49.725 | 18.717 | 53.130 | 1.00 | 72.65 | 8 |
| | ATOM | 1015 | N VAL A 128 | 48.572 | 20.463 | 52.317 | 1.00 | 72.58 | 7 |
| 55 | ATOM | 1016 | CA VAL A 128 | 49.779 | 21.109 | 51.830 | 1.00 | 73.82 | 6 |
| | ATOM | 1017 | CB VAL A 128 | 49.505 | 22.482 | 51.162 | 1.00 | 73.07 | 6 |
| | ATOM | 1018 | CG1 VAL A 128 | 48.855 | 22.272 | 49.837 | 1.00 | 75.57 | 6 |
| | ATOM | 1019 | CG2 VAL A 128 | 48.625 | 23.359 | 52.065 | 1.00 | 72.32 | 6 |
| | ATOM | 1020 | C VAL A 128 | 50.792 | 21.376 | 52.912 | 1.00 | 75.60 | 6 |
| 60 | ATOM | 1021 | O VAL A 128 | 51.984 | 21.102 | 52.727 | 1.00 | 76.00 | 8 |
| | ATOM | 1022 | N ASP A 129 | 50.324 | 21.907 | 54.041 | 1.00 | 77.55 | 7 |
| | ATOM | 1023 | CA ASP A 129 | 51.241 | 22.287 | 55.107 | 1.00 | 79.65 | 6 |
| | ATOM | 1024 | CB ASP A 129 | 50.507 | 23.015 | 56.235 | 1.00 | 79.08 | 6 |
| | ATOM | 1025 | CG ASP A 129 | 51.427 | 23.954 | 57.017 | 1.00 | 80.06 | 6 |
| | ATOM | 1026 | OD1 ASP A 129 | 51.000 | 25.097 | 57.338 | 1.00 | 80.12 | 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 1027 | OD2 | ASP | A | 129 | 52.578 | 23.546 | 57.311 | 1.00 | 80.59 | 8 |
| | ATOM | 1028 | C | ASP | A | 129 | 52.085 | 21.164 | 55.676 | 1.00 | 80.77 | 6 |
| | ATOM | 1029 | O | ASP | A | 129 | 53.089 | 21.441 | 56.355 | 1.00 | 80.25 | 8 |
| | ATOM | 1030 | N | THR | A | 130 | 51.724 | 19.907 | 55.389 | 1.00 | 80.58 | 7 |
| 5 | ATOM | 1031 | CA | THR | A | 130 | 52.541 | 18.824 | 55.925 | 1.00 | 81.44 | 6 |
| | ATOM | 1032 | CB | THR | A | 130 | 52.508 | 18.858 | 57.465 | 1.00 | 83.89 | 6 |
| | ATOM | 1033 | OG1 | THR | A | 130 | 51.433 | 19.722 | 57.880 | 1.00 | 85.49 | 8 |
| | ATOM | 1034 | CG2 | THR | A | 130 | 53.882 | 19.331 | 58.047 | 1.00 | 83.12 | 6 |
| 10 | ATOM | 1035 | C | THR | A | 130 | 52.309 | 17.374 | 55.529 | 1.00 | 80.12 | 6 |
| | ATOM | 1036 | O | THR | A | 130 | 51.199 | 16.974 | 55.148 | 1.00 | 78.43 | 8 |
| | ATOM | 1037 | N | GLU | A | 131 | 53.404 | 16.611 | 55.654 | 1.00 | 79.90 | 7 |
| | ATOM | 1038 | CA | GLU | A | 131 | 53.459 | 15.165 | 55.432 | 1.00 | 80.19 | 6 |
| | ATOM | 1039 | CB | GLU | A | 131 | 52.364 | 14.489 | 56.272 | 1.00 | 82.93 | 6 |
| | ATOM | 1040 | CG | GLU | A | 131 | 52.693 | 14.372 | 57.760 | 1.00 | 86.59 | 6 |
| 15 | ATOM | 1041 | CD | GLU | A | 131 | 51.440 | 14.289 | 58.632 | 1.00 | 88.67 | 6 |
| | ATOM | 1042 | OE1 | GLU | A | 131 | 50.524 | 13.470 | 58.311 | 1.00 | 89.43 | 8 |
| | ATOM | 1043 | OE2 | GLU | A | 131 | 51.380 | 15.050 | 59.638 | 1.00 | 88.79 | 8 |
| | ATOM | 1044 | C | GLU | A | 131 | 53.378 | 14.637 | 54.012 | 1.00 | 79.05 | 6 |
| 20 | ATOM | 1045 | O | GLU | A | 131 | 54.337 | 14.716 | 53.231 | 1.00 | 77.86 | 8 |
| | ATOM | 1046 | N | SER | A | 132 | 52.227 | 14.033 | 53.727 | 1.00 | 77.68 | 7 |
| | ATOM | 1047 | CA | SER | A | 132 | 51.915 | 13.474 | 52.426 | 1.00 | 76.46 | 6 |
| | ATOM | 1048 | CB | SER | A | 132 | 50.796 | 12.429 | 52.576 | 1.00 | 76.05 | 6 |
| | ATOM | 1049 | OG | SER | A | 132 | 49.642 | 12.990 | 53.176 | 1.00 | 74.46 | 8 |
| | ATOM | 1050 | C | SER | A | 132 | 51.462 | 14.653 | 51.533 | 1.00 | 75.70 | 6 |
| 25 | ATOM | 1051 | O | SER | A | 132 | 51.123 | 14.479 | 50.355 | 1.00 | 75.58 | 8 |
| | ATOM | 1052 | N | GLY | A | 133 | 51.468 | 15.848 | 52.127 | 1.00 | 73.94 | 7 |
| | ATOM | 1053 | CA | GLY | A | 133 | 51.094 | 17.056 | 51.421 | 1.00 | 71.52 | 6 |
| | ATOM | 1054 | C | GLY | A | 133 | 49.754 | 16.971 | 50.735 | 1.00 | 70.11 | 6 |
| 30 | ATOM | 1055 | O | GLY | A | 133 | 48.927 | 16.115 | 51.060 | 1.00 | 69.95 | 8 |
| | ATOM | 1056 | N | ALA | A | 134 | 49.540 | 17.864 | 49.774 | 1.00 | 68.35 | 7 |
| | ATOM | 1057 | CA | ALA | A | 134 | 48.290 | 17.895 | 49.033 | 1.00 | 65.73 | 6 |
| | ATOM | 1058 | CB | ALA | A | 134 | 47.748 | 19.321 | 48.982 | 1.00 | 65.87 | 6 |
| | ATOM | 1059 | C | ALA | A | 134 | 48.476 | 17.359 | 47.621 | 1.00 | 63.96 | 6 |
| | ATOM | 1060 | O | ALA | A | 134 | 49.600 | 17.219 | 47.124 | 1.00 | 61.93 | 8 |
| 35 | ATOM | 1061 | N | THR | A | 135 | 47.353 | 17.048 | 46.985 | 1.00 | 63.38 | 7 |
| | ATOM | 1062 | CA | THR | A | 135 | 47.359 | 16.549 | 45.621 | 1.00 | 62.44 | 6 |
| | ATOM | 1063 | CB | THR | A | 135 | 47.003 | 15.066 | 45.562 | 1.00 | 62.52 | 6 |
| | ATOM | 1064 | OG1 | THR | A | 135 | 47.951 | 14.323 | 46.345 | 1.00 | 62.25 | 8 |
| | ATOM | 1065 | CG2 | THR | A | 135 | 47.040 | 14.574 | 44.122 | 1.00 | 61.31 | 6 |
| 40 | ATOM | 1066 | C | THR | A | 135 | 46.350 | 17.355 | 44.820 | 1.00 | 61.68 | 6 |
| | ATOM | 1067 | O | THR | A | 135 | 45.120 | 17.188 | 44.944 | 1.00 | 60.36 | 8 |
| | ATOM | 1068 | N | CYS | A | 136 | 46.900 | 18.259 | 44.017 | 1.00 | 59.30 | 7 |
| | ATOM | 1069 | CA | CYS | A | 136 | 46.115 | 19.129 | 43.178 | 1.00 | 56.11 | 6 |
| | ATOM | 1070 | C | CYS | A | 136 | 46.111 | 18.538 | 41.778 | 1.00 | 55.58 | 6 |
| 45 | ATOM | 1071 | O | CYS | A | 136 | 47.168 | 18.370 | 41.163 | 1.00 | 53.10 | 8 |
| | ATOM | 1072 | CB | CYS | A | 136 | 46.739 | 20.518 | 43.181 | 1.00 | 55.44 | 6 |
| | ATOM | 1073 | SG | CYS | A | 136 | 46.010 | 21.663 | 41.978 | 1.00 | 54.51 | 16 |
| | ATOM | 1074 | N | ARG | A | 137 | 44.917 | 18.191 | 41.298 | 1.00 | 55.48 | 7 |
| | ATOM | 1075 | CA | ARG | A | 137 | 44.764 | 17.611 | 39.968 | 1.00 | 56.07 | 6 |
| 50 | ATOM | 1076 | CB | ARG | A | 137 | 43.786 | 16.431 | 39.990 | 1.00 | 58.27 | 6 |
| | ATOM | 1077 | CG | ARG | A | 137 | 44.213 | 15.318 | 40.915 | 1.00 | 62.94 | 6 |
| | ATOM | 1078 | CD | ARG | A | 137 | 43.017 | 14.517 | 41.384 | 1.00 | 67.01 | 6 |
| | ATOM | 1079 | NE | ARG | A | 137 | 43.308 | 13.821 | 42.641 | 1.00 | 72.70 | 7 |
| | ATOM | 1080 | CZ | ARG | A | 137 | 44.131 | 12.772 | 42.762 | 1.00 | 74.69 | 6 |
| 55 | ATOM | 1081 | NH1 | ARG | A | 137 | 44.765 | 12.270 | 41.696 | 1.00 | 74.12 | 7 |
| | ATOM | 1082 | NH2 | ARG | A | 137 | 44.326 | 12.226 | 43.958 | 1.00 | 74.27 | 7 |
| | ATOM | 1083 | C | ARG | A | 137 | 44.265 | 18.670 | 39.010 | 1.00 | 53.72 | 6 |
| | ATOM | 1084 | O | ARG | A | 137 | 43.325 | 19.396 | 39.301 | 1.00 | 51.52 | 8 |
| | ATOM | 1085 | N | ILE | A | 138 | 44.917 | 18.738 | 37.860 | 1.00 | 52.05 | 7 |
| 60 | ATOM | 1086 | CA | ILE | A | 138 | 44.582 | 19.696 | 36.825 | 1.00 | 50.25 | 6 |
| | ATOM | 1087 | CB | ILE | A | 138 | 45.778 | 20.624 | 36.557 | 1.00 | 49.78 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1088 | CG2 | ILE | A | 138 | 45.449 | 21.566 | 35.421 | 1.00 | 48.31 | 6 |
| | ATOM | 1089 | CG1 | ILE | A | 138 | 46.150 | 21.389 | 37.837 | 1.00 | 48.07 | 6 |
| | ATOM | 1090 | CD1 | ILE | A | 138 | 47.444 | 22.144 | 37.750 | 1.00 | 41.58 | 6 |
| | ATOM | 1091 | C | ILE | A | 138 | 44.270 | 18.925 | 35.555 | 1.00 | 49.76 | 6 |
| 5 | ATOM | 1092 | O | ILE | A | 138 | 45.119 | 18.190 | 35.058 | 1.00 | 50.40 | 8 |
| | ATOM | 1093 | N | LYS | A | 139 | 43.059 | 19.081 | 35.032 | 1.00 | 49.44 | 7 |
| | ATOM | 1094 | CA | LYS | A | 139 | 42.672 | 18.374 | 33.809 | 1.00 | 51.81 | 6 |
| | ATOM | 1095 | CB | LYS | A | 139 | 41.285 | 17.713 | 33.969 | 1.00 | 52.86 | 6 |
| | ATOM | 1096 | CG | LYS | A | 139 | 41.176 | 16.772 | 35.164 | 1.00 | 56.41 | 6 |
| 10 | ATOM | 1097 | CD | LYS | A | 139 | 39.919 | 15.940 | 35.137 | 1.00 | 57.01 | 6 |
| | ATOM | 1098 | CE | LYS | A | 139 | 39.978 | 14.888 | 34.047 | 1.00 | 60.31 | 6 |
| | ATOM | 1099 | NZ | LYS | A | 139 | 38.728 | 14.066 | 33.965 | 1.00 | 59.02 | 7 |
| | ATOM | 1100 | C | LYS | A | 139 | 42.628 | 19.317 | 32.615 | 1.00 | 51.20 | 6 |
| | ATOM | 1101 | O | LYS | A | 139 | 41.964 | 20.340 | 32.673 | 1.00 | 51.87 | 8 |
| 15 | ATOM | 1102 | N | ILE | A | 140 | 43.325 | 18.979 | 31.535 | 1.00 | 49.23 | 7 |
| | ATOM | 1103 | CA | ILE | A | 140 | 43.295 | 19.826 | 30.354 | 1.00 | 49.38 | 6 |
| | ATOM | 1104 | CB | ILE | A | 140 | 44.578 | 20.710 | 30.278 | 1.00 | 50.36 | 6 |
| | ATOM | 1105 | CG2 | ILE | A | 140 | 44.889 | 21.277 | 31.653 | 1.00 | 51.45 | 6 |
| | ATOM | 1106 | CG1 | ILE | A | 140 | 45.794 | 19.900 | 29.868 | 1.00 | 50.82 | 6 |
| 20 | ATOM | 1107 | CD1 | ILE | A | 140 | 47.103 | 20.630 | 30.148 | 1.00 | 51.49 | 6 |
| | ATOM | 1108 | C | ILE | A | 140 | 43.088 | 19.025 | 29.066 | 1.00 | 47.91 | 6 |
| | ATOM | 1109 | O | ILE | A | 140 | 43.721 | 18.006 | 28.859 | 1.00 | 46.67 | 8 |
| | ATOM | 1110 | N | GLY | A | 141 | 42.168 | 19.485 | 28.220 | 1.00 | 48.53 | 7 |
| | ATOM | 1111 | CA | GLY | A | 141 | 41.885 | 18.811 | 26.959 | 1.00 | 47.60 | 6 |
| 25 | ATOM | 1112 | C | GLY | A | 141 | 41.255 | 19.765 | 25.958 | 1.00 | 48.49 | 6 |
| | ATOM | 1113 | O | GLY | A | 141 | 40.938 | 20.900 | 26.317 | 1.00 | 49.03 | 8 |
| | ATOM | 1114 | N | SER | A | 142 | 41.070 | 19.329 | 24.712 | 1.00 | 46.01 | 7 |
| | ATOM | 1115 | CA | SER | A | 142 | 40.466 | 20.195 | 23.699 | 1.00 | 43.95 | 6 |
| | ATOM | 1116 | CB | SER | A | 142 | 40.306 | 19.466 | 22.370 | 1.00 | 44.36 | 6 |
| 30 | ATOM | 1117 | OG | SER | A | 142 | 39.494 | 20.214 | 21.477 | 1.00 | 39.73 | 8 |
| | ATOM | 1118 | C | SER | A | 142 | 39.107 | 20.686 | 24.144 | 1.00 | 45.09 | 6 |
| | ATOM | 1119 | O | SER | A | 142 | 38.319 | 19.934 | 24.714 | 1.00 | 47.13 | 8 |
| | ATOM | 1120 | N | TRP | A | 143 | 38.822 | 21.947 | 23.862 | 1.00 | 43.97 | 7 |
| | ATOM | 1121 | CA | TRP | A | 143 | 37.564 | 22.537 | 24.256 | 1.00 | 41.28 | 6 |
| 35 | ATOM | 1122 | CB | TRP | A | 143 | 37.754 | 24.033 | 24.473 | 1.00 | 42.28 | 6 |
| | ATOM | 1123 | CG | TRP | A | 143 | 36.577 | 24.697 | 25.126 | 1.00 | 42.52 | 6 |
| | ATOM | 1124 | CD2 | TRP | A | 143 | 36.215 | 24.610 | 26.505 | 1.00 | 39.43 | 6 |
| | ATOM | 1125 | CE2 | TRP | A | 143 | 35.025 | 25.359 | 26.676 | 1.00 | 39.15 | 6 |
| | ATOM | 1126 | CE3 | TRP | A | 143 | 36.778 | 23.969 | 27.613 | 1.00 | 37.16 | 6 |
| 40 | ATOM | 1127 | CD1 | TRP | A | 143 | 35.618 | 25.480 | 24.526 | 1.00 | 41.93 | 6 |
| | ATOM | 1128 | NE1 | TRP | A | 143 | 34.681 | 25.880 | 25.456 | 1.00 | 40.50 | 7 |
| | ATOM | 1129 | CZ2 | TRP | A | 143 | 34.393 | 25.480 | 27.911 | 1.00 | 39.06 | 6 |
| | ATOM | 1130 | CZ3 | TRP | A | 143 | 36.150 | 24.090 | 28.837 | 1.00 | 39.37 | 6 |
| | ATOM | 1131 | CH2 | TRP | A | 143 | 34.968 | 24.840 | 28.978 | 1.00 | 39.40 | 6 |
| 45 | ATOM | 1132 | C | TRP | A | 143 | 36.450 | 22.307 | 23.258 | 1.00 | 41.37 | 6 |
| | ATOM | 1133 | O | TRP | A | 143 | 35.287 | 22.239 | 23.632 | 1.00 | 42.45 | 8 |
| | ATOM | 1134 | N | THR | A | 144 | 36.790 | 22.179 | 21.983 | 1.00 | 41.97 | 7 |
| | ATOM | 1135 | CA | THR | A | 144 | 35.760 | 21.992 | 20.979 | 1.00 | 41.13 | 6 |
| | ATOM | 1136 | CB | THR | A | 144 | 35.703 | 23.191 | 20.051 | 1.00 | 39.00 | 6 |
| 50 | ATOM | 1137 | OG1 | THR | A | 144 | 36.994 | 23.416 | 19.490 | 1.00 | 39.19 | 8 |
| | ATOM | 1138 | CG2 | THR | A | 144 | 35.288 | 24.420 | 20.818 | 1.00 | 37.78 | 6 |
| | ATOM | 1139 | C | THR | A | 144 | 35.879 | 20.738 | 20.148 | 1.00 | 42.54 | 6 |
| | ATOM | 1140 | O | THR | A | 144 | 34.941 | 20.385 | 19.443 | 1.00 | 45.82 | 8 |
| | ATOM | 1141 | N | HIS | A | 145 | 37.012 | 20.054 | 20.233 | 1.00 | 43.18 | 7 |
| 55 | ATOM | 1142 | CA | HIS | A | 145 | 37.187 | 18.837 | 19.459 | 1.00 | 46.20 | 6 |
| | ATOM | 1143 | CB | HIS | A | 145 | 38.517 | 18.875 | 18.707 | 1.00 | 46.05 | 6 |
| | ATOM | 1144 | CG | HIS | A | 145 | 38.588 | 19.933 | 17.646 | 1.00 | 46.56 | 6 |
| | ATOM | 1145 | CD2 | HIS | A | 145 | 37.994 | 20.022 | 16.432 | 1.00 | 45.44 | 6 |
| | ATOM | 1146 | ND1 | HIS | A | 145 | 39.366 | 21.061 | 17.772 | 1.00 | 44.61 | 7 |
| 60 | ATOM | 1147 | CE1 | HIS | A | 145 | 39.250 | 21.797 | 16.682 | 1.00 | 43.87 | 6 |
| | ATOM | 1148 | NE2 | HIS | A | 145 | 38.423 | 21.189 | 15.853 | 1.00 | 41.35 | 7 |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1149 | C HIS A 145 | 37.105 | 17.570 | 20.303 | 1.00 | 47.36 | 6 |
| | ATOM | 1150 | O HIS A 145 | 37.811 | 17.422 | 21.298 | 1.00 | 47.71 | 8 |
| | ATOM | 1151 | N HIS A 146 | 36.230 | 16.656 | 19.898 | 1.00 | 48.75 | 7 |
| | ATOM | 1152 | CA HIS A 146 | 36.067 | 15.400 | 20.609 | 1.00 | 50.47 | 6 |
| | ATOM | 1153 | CB HIS A 146 | 34.658 | 14.846 | 20.365 | 1.00 | 49.28 | 6 |
| 10 | ATOM | 1154 | CG HIS A 146 | 34.314 | 14.694 | 18.919 | 1.00 | 50.42 | 6 |
| | ATOM | 1155 | CD2 HIS A 146 | 34.954 | 14.057 | 17.910 | 1.00 | 50.68 | 6 |
| | ATOM | 1156 | ND1 HIS A 146 | 33.183 | 15.248 | 18.362 | 1.00 | 51.90 | 7 |
| | ATOM | 1157 | CE1 HIS A 146 | 33.138 | 14.962 | 17.073 | 1.00 | 49.57 | 6 |
| | ATOM | 1158 | NE2 HIS A 146 | 34.202 | 14.239 | 16.774 | 1.00 | 51.03 | 7 |
| 15 | ATOM | 1159 | C HIS A 146 | 37.137 | 14.396 | 20.167 | 1.00 | 49.74 | 6 |
| | ATOM | 1160 | O HIS A 146 | 37.927 | 14.673 | 19.268 | 1.00 | 49.87 | 8 |
| | ATOM | 1161 | N SER A 147 | 37.145 | 13.234 | 20.809 | 1.00 | 50.23 | 7 |
| | ATOM | 1162 | CA SER A 147 | 38.101 | 12.158 | 20.543 | 1.00 | 50.98 | 6 |
| | ATOM | 1163 | CB SER A 147 | 37.722 | 10.934 | 21.372 | 1.00 | 50.73 | 6 |
| 20 | ATOM | 1164 | OG SER A 147 | 36.346 | 10.642 | 21.240 | 1.00 | 51.84 | 8 |
| | ATOM | 1165 | C SER A 147 | 38.314 | 11.730 | 19.096 | 1.00 | 51.53 | 6 |
| | ATOM | 1166 | O SER A 147 | 39.374 | 11.228 | 18.754 | 1.00 | 50.53 | 8 |
| | ATOM | 1167 | N ARG A 148 | 37.319 | 11.925 | 18.245 | 1.00 | 53.75 | 7 |
| | ATOM | 1168 | CA ARG A 148 | 37.444 | 11.528 | 16.850 | 1.00 | 56.68 | 6 |
| 25 | ATOM | 1169 | CB ARG A 148 | 36.052 | 11.408 | 16.221 | 1.00 | 60.77 | 6 |
| | ATOM | 1170 | CG ARG A 148 | 35.100 | 10.487 | 16.985 | 1.00 | 70.28 | 6 |
| | ATOM | 1171 | CD ARG A 148 | 33.673 | 10.516 | 16.423 | 1.00 | 76.18 | 6 |
| | ATOM | 1172 | NE ARG A 148 | 32.702 | 9.919 | 17.351 | 1.00 | 83.11 | 7 |
| | ATOM | 1173 | CZ ARG A 148 | 32.685 | 8.632 | 17.719 | 1.00 | 85.65 | 6 |
| 30 | ATOM | 1174 | NH1 ARG A 148 | 33.595 | 7.781 | 17.243 | 1.00 | 86.70 | 7 |
| | ATOM | 1175 | NH2 ARG A 148 | 31.746 | 8.187 | 18.549 | 1.00 | 85.60 | 7 |
| | ATOM | 1176 | C ARG A 148 | 38.295 | 12.502 | 16.025 | 1.00 | 56.73 | 6 |
| | ATOM | 1177 | O ARG A 148 | 38.774 | 12.157 | 14.938 | 1.00 | 56.48 | 8 |
| | ATOM | 1178 | N GLU A 149 | 38.477 | 13.714 | 16.553 | 1.00 | 55.77 | 7 |
| 35 | ATOM | 1179 | CA GLU A 149 | 39.233 | 14.767 | 15.884 | 1.00 | 51.96 | 6 |
| | ATOM | 1180 | CB GLU A 149 | 38.384 | 16.037 | 15.821 | 1.00 | 52.02 | 6 |
| | ATOM | 1181 | CG GLU A 149 | 36.918 | 15.748 | 15.527 | 1.00 | 51.38 | 6 |
| | ATOM | 1182 | CD GLU A 149 | 36.065 | 16.989 | 15.423 | 1.00 | 49.98 | 6 |
| | ATOM | 1183 | OE1 GLU A 149 | 36.220 | 17.879 | 16.273 | 1.00 | 50.58 | 8 |
| 40 | ATOM | 1184 | OE2 GLU A 149 | 35.226 | 17.070 | 14.506 | 1.00 | 46.84 | 8 |
| | ATOM | 1185 | C GLU A 149 | 40.531 | 15.030 | 16.627 | 1.00 | 50.15 | 6 |
| | ATOM | 1186 | O GLU A 149 | 41.584 | 15.167 | 16.013 | 1.00 | 49.33 | 8 |
| | ATOM | 1187 | N ILE A 150 | 40.454 | 15.100 | 17.950 | 1.00 | 47.25 | 7 |
| | ATOM | 1188 | CA ILE A 150 | 41.643 | 15.309 | 18.748 | 1.00 | 48.44 | 6 |
| 45 | ATOM | 1189 | CB ILE A 150 | 41.712 | 16.740 | 19.374 | 1.00 | 48.83 | 6 |
| | ATOM | 1190 | CG2 ILE A 150 | 42.759 | 16.793 | 20.481 | 1.00 | 44.42 | 6 |
| | ATOM | 1191 | CG1 ILE A 150 | 42.104 | 17.769 | 18.316 | 1.00 | 49.22 | 6 |
| | ATOM | 1192 | CD1 ILE A 150 | 42.185 | 19.175 | 18.839 | 1.00 | 45.68 | 6 |
| | ATOM | 1193 | C ILE A 150 | 41.707 | 14.310 | 19.881 | 1.00 | 50.37 | 6 |
| 50 | ATOM | 1194 | O ILE A 150 | 40.712 | 14.031 | 20.536 | 1.00 | 50.37 | 8 |
| | ATOM | 1195 | N SER A 151 | 42.902 | 13.781 | 20.104 | 1.00 | 52.48 | 7 |
| | ATOM | 1196 | CA SER A 151 | 43.156 | 12.841 | 21.178 | 1.00 | 54.49 | 6 |
| | ATOM | 1197 | CB SER A 151 | 43.437 | 11.452 | 20.611 | 1.00 | 54.22 | 6 |
| | ATOM | 1198 | OG SER A 151 | 44.619 | 11.457 | 19.844 | 1.00 | 54.28 | 8 |
| 55 | ATOM | 1199 | C SER A 151 | 44.385 | 13.381 | 21.899 | 1.00 | 55.57 | 6 |
| | ATOM | 1200 | O SER A 151 | 45.347 | 13.798 | 21.257 | 1.00 | 56.29 | 8 |
| | ATOM | 1201 | N VAL A 152 | 44.337 | 13.400 | 23.227 | 1.00 | 57.03 | 7 |
| | ATOM | 1202 | CA VAL A 152 | 45.447 | 13.897 | 24.033 | 1.00 | 59.85 | 6 |
| | ATOM | 1203 | CB VAL A 152 | 44.979 | 14.922 | 25.100 | 1.00 | 59.80 | 6 |
| 60 | ATOM | 1204 | CG1 VAL A 152 | 44.170 | 16.021 | 24.447 | 1.00 | 60.14 | 6 |
| | ATOM | 1205 | CG2 VAL A 152 | 44.163 | 14.225 | 26.175 | 1.00 | 61.09 | 6 |
| | ATOM | 1206 | C VAL A 152 | 46.084 | 12.722 | 24.747 | 1.00 | 61.00 | 6 |
| | ATOM | 1207 | O VAL A 152 | 45.393 | 11.785 | 25.132 | 1.00 | 59.83 | 8 |
| | ATOM | 1208 | N ASP A 153 | 47.398 | 12.780 | 24.932 | 1.00 | 63.57 | 7 |
| | ATOM | 1209 | CA ASP A 153 | 48.114 | 11.690 | 25.582 | 1.00 | 66.72 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|--------|---|--|
| 5 | ATOM | 1210 | CB | ASP A 153 | 48.620 | 10.724 | 24.505 | 1.00 | 66.16 | 6 | |
| | ATOM | 1211 | CG | ASP A 153 | 47.505 | 10.245 | 23.573 | 1.00 | 67.72 | 6 | |
| | ATOM | 1212 | OD1 | ASP A 153 | 46.769 | 9.317 | 23.972 | 1.00 | 68.96 | 8 | |
| | ATOM | 1213 | OD2 | ASP A 153 | 47.354 | 10.801 | 22.451 | 1.00 | 67.60 | 8 | |
| | ATOM | 1214 | C | ASP A 153 | 49.293 | 12.198 | 26.422 | 1.00 | 68.93 | 6 | |
| 10 | ATOM | 1215 | O | ASP A 153 | 49.951 | 13.175 | 26.058 | 1.00 | 69.39 | 8 | |
| | ATOM | 1216 | N | PRO A 154 | 49.553 | 11.564 | 27.577 | 1.00 | 70.74 | 7 | |
| | ATOM | 1217 | CD | PRO A 154 | 48.601 | 10.759 | 28.357 | 1.00 | 71.40 | 6 | |
| | ATOM | 1218 | CA | PRO A 154 | 50.675 | 11.995 | 28.421 | 1.00 | 73.42 | 6 | |
| | ATOM | 1219 | CB | PRO A 154 | 50.421 | 11.266 | 29.735 | 1.00 | 72.22 | 6 | |
| 15 | ATOM | 1220 | CG | PRO A 154 | 48.930 | 11.182 | 29.776 | 1.00 | 72.97 | 6 | |
| | ATOM | 1221 | C | PRO A 154 | 51.999 | 11.580 | 27.773 | 1.00 | 75.99 | 6 | |
| | ATOM | 1222 | O | PRO A 154 | 51.997 | 10.951 | 26.716 | 1.00 | 75.49 | 8 | |
| | ATOM | 1223 | N | THR A 155 | 53.121 | 11.916 | 28.406 | 1.00 | 79.97 | 7 | |
| | ATOM | 1224 | CA | THR A 155 | 54.433 | 11.580 | 27.851 | 1.00 | 84.54 | 6 | |
| 20 | ATOM | 1225 | CB | THR A 155 | 55.002 | 12.797 | 27.084 | 1.00 | 84.38 | 6 | |
| | ATOM | 1226 | OG1 | THR A 155 | 55.314 | 13.844 | 28.015 | 1.00 | 85.24 | 8 | |
| | ATOM | 1227 | CG2 | THR A 155 | 53.979 | 13.326 | 26.085 | 1.00 | 83.86 | 6 | |
| | ATOM | 1228 | C | THR A 155 | 55.504 | 11.101 | 28.868 | 1.00 | 88.31 | 6 | |
| | ATOM | 1229 | O | THR A 155 | 55.179 | 10.480 | 29.905 | 1.00 | 89.23 | 8 | |
| 25 | ATOM | 1230 | N | THR A 156 | 56.774 | 11.402 | 28.539 | 1.00 | 91.22 | 7 | |
| | ATOM | 1231 | CA | THR A 156 | 57.970 | 11.057 | 29.337 | 1.00 | 93.64 | 6 | |
| | ATOM | 1232 | CB | THR A 156 | 59.146 | 12.041 | 29.041 | 1.00 | 93.80 | 6 | |
| | ATOM | 1233 | OG1 | THR A 156 | 59.430 | 12.048 | 27.631 | 1.00 | 93.55 | 8 | |
| | ATOM | 1234 | CG2 | THR A 156 | 60.414 | 11.624 | 29.839 | 1.00 | 93.12 | 6 | |
| 30 | ATOM | 1235 | C | THR A 156 | 57.778 | 11.031 | 30.862 | 1.00 | 95.49 | 6 | |
| | ATOM | 1236 | O | THR A 156 | 57.812 | 12.080 | 31.532 | 1.00 | 95.50 | 8 | |
| | ATOM | 1237 | N | GLU A 157 | 57.614 | 9.827 | 31.406 | 1.00 | 97.12 | 7 | |
| | ATOM | 1238 | CA | GLU A 157 | 57.411 | 9.649 | 32.841 | 1.00 | 98.24 | 6 | |
| | ATOM | 1239 | CB | GLU A 157 | 56.619 | 8.370 | 33.095 | 1.00 | 100.23 | 6 | |
| 35 | ATOM | 1240 | CG | GLU A 157 | 55.476 | 8.150 | 32.109 | 1.00 | 103.23 | 6 | |
| | ATOM | 1241 | CD | GLU A 157 | 54.728 | 6.842 | 32.372 | 1.00 | 104.38 | 6 | |
| | ATOM | 1242 | OE1 | GLU A 157 | 55.391 | 5.769 | 32.462 | 1.00 | 103.49 | 8 | |
| | ATOM | 1243 | OE2 | GLU A 157 | 53.475 | 6.896 | 32.482 | 1.00 | 105.11 | 8 | |
| | ATOM | 1244 | C | GLU A 157 | 58.731 | 9.570 | 33.591 | 1.00 | 98.22 | 6 | |
| 40 | ATOM | 1245 | O | GLU A 157 | 58.742 | 9.488 | 34.825 | 1.00 | 98.77 | 8 | |
| | ATOM | 1246 | N | ASN A 158 | 59.840 | 9.582 | 32.854 | 1.00 | 97.95 | 7 | |
| | ATOM | 1247 | CA | ASN A 158 | 61.154 | 9.505 | 33.494 | 1.00 | 98.34 | 6 | |
| | ATOM | 1248 | CB | ASN A 158 | 62.244 | 9.212 | 32.455 | 1.00 | 100.52 | 6 | |
| | ATOM | 1249 | CG | ASN A 158 | 61.953 | 7.969 | 31.634 | 1.00 | 102.32 | 6 | |
| 45 | ATOM | 1250 | OD1 | ASN A 158 | 61.787 | 6.872 | 32.184 | 1.00 | 104.16 | 8 | |
| | ATOM | 1251 | ND2 | ASN A 158 | 61.898 | 8.131 | 30.305 | 1.00 | 102.61 | 7 | |
| | ATOM | 1252 | C | ASN A 158 | 61.471 | 10.832 | 34.196 | 1.00 | 97.02 | 6 | |
| | ATOM | 1253 | O | ASN A 158 | 61.170 | 11.019 | 35.392 | 1.00 | 96.34 | 8 | |
| | ATOM | 1254 | N | SER A 159 | 62.093 | 11.729 | 33.423 | 1.00 | 94.95 | 7 | |
| 50 | ATOM | 1255 | CA | SER A 159 | 62.492 | 13.069 | 33.857 | 1.00 | 91.51 | 6 | |
| | ATOM | 1256 | CB | SER A 159 | 61.878 | 14.091 | 32.890 | 1.00 | 91.99 | 6 | |
| | ATOM | 1257 | OG | SER A 159 | 60.550 | 13.708 | 32.529 | 1.00 | 90.83 | 8 | |
| | ATOM | 1258 | C | SER A 159 | 62.116 | 13.412 | 35.301 | 1.00 | 88.77 | 6 | |
| | ATOM | 1259 | O | SER A 159 | 60.939 | 13.380 | 35.666 | 1.00 | 88.38 | 8 | |
| 55 | ATOM | 1260 | N | ASP A 160 | 63.120 | 13.728 | 36.120 | 1.00 | 85.60 | 7 | |
| | ATOM | 1261 | CA | ASP A 160 | 62.867 | 14.093 | 37.517 | 1.00 | 81.69 | 6 | |
| | ATOM | 1262 | CB | ASP A 160 | 64.107 | 14.716 | 38.164 | 1.00 | 81.79 | 6 | |
| | ATOM | 1263 | CG | ASP A 160 | 63.827 | 15.217 | 39.578 | 1.00 | 82.16 | 6 | |
| | ATOM | 1264 | OD1 | ASP A 160 | 64.609 | 16.057 | 40.075 | 1.00 | 82.93 | 8 | |
| 60 | ATOM | 1265 | OD2 | ASP A 160 | 62.824 | 14.766 | 40.194 | 1.00 | 81.33 | 8 | |
| | ATOM | 1266 | C | ASP A 160 | 61.748 | 15.125 | 37.556 | 1.00 | 78.87 | 6 | |
| | ATOM | 1267 | O | ASP A 160 | 61.906 | 16.215 | 36.997 | 1.00 | 77.29 | 8 | |
| | ATOM | 1268 | N | ASP A 161 | 60.643 | 14.783 | 38.223 | 1.00 | 75.12 | 7 | |
| | ATOM | 1269 | CA | ASP A 161 | 59.493 | 15.677 | 38.324 | 1.00 | 71.64 | 6 | |
| | ATOM | 1270 | CB | ASP A 161 | 58.433 | 15.111 | 39.273 | 1.00 | 71.12 | 6 | |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1271 | CG | ASP | A | 161 | 57.719 | 13.895 | 38.698 | 1.00 | 71.43 | 6 |
| | ATOM | 1272 | OD1 | ASP | A | 161 | 57.509 | 13.854 | 37.463 | 1.00 | 70.50 | 8 |
| | ATOM | 1273 | OD2 | ASP | A | 161 | 57.353 | 12.983 | 39.480 | 1.00 | 71.76 | 8 |
| | ATOM | 1274 | C | ASP | A | 161 | 59.814 | 17.097 | 38.756 | 1.00 | 69.97 | 6 |
| 5 | ATOM | 1275 | O | ASP | A | 161 | 59.009 | 18.001 | 38.545 | 1.00 | 69.41 | 8 |
| | ATOM | 1276 | N | SER | A | 162 | 60.974 | 17.321 | 39.358 | 1.00 | 68.43 | 7 |
| | ATOM | 1277 | CA | SER | A | 162 | 61.282 | 18.682 | 39.774 | 1.00 | 68.46 | 6 |
| | ATOM | 1278 | CB | SER | A | 162 | 61.190 | 18.809 | 41.308 | 1.00 | 68.76 | 6 |
| | ATOM | 1279 | OG | SER | A | 162 | 62.209 | 18.069 | 41.962 | 1.00 | 68.11 | 8 |
| 10 | ATOM | 1280 | C | SER | A | 162 | 62.636 | 19.163 | 39.289 | 1.00 | 67.78 | 6 |
| | ATOM | 1281 | O | SER | A | 162 | 63.264 | 20.014 | 39.917 | 1.00 | 67.84 | 8 |
| | ATOM | 1282 | N | GLU | A | 163 | 63.087 | 18.640 | 38.156 | 1.00 | 67.60 | 7 |
| | ATOM | 1283 | CA | GLU | A | 163 | 64.382 | 19.052 | 37.649 | 1.00 | 68.35 | 6 |
| | ATOM | 1284 | CB | GLU | A | 163 | 64.884 | 18.051 | 36.609 | 1.00 | 70.48 | 6 |
| 15 | ATOM | 1285 | CG | GLU | A | 163 | 64.380 | 18.242 | 35.193 | 1.00 | 73.24 | 6 |
| | ATOM | 1286 | CD | GLU | A | 163 | 65.111 | 17.328 | 34.204 | 1.00 | 75.50 | 6 |
| | ATOM | 1287 | OE1 | GLU | A | 163 | 64.835 | 16.097 | 34.211 | 1.00 | 76.99 | 8 |
| | ATOM | 1288 | OE2 | GLU | A | 163 | 65.970 | 17.842 | 33.438 | 1.00 | 73.24 | 8 |
| | ATOM | 1289 | C | GLU | A | 163 | 64.342 | 20.475 | 37.083 | 1.00 | 68.50 | 6 |
| 20 | ATOM | 1290 | O | GLU | A | 163 | 65.385 | 21.062 | 36.774 | 1.00 | 69.25 | 8 |
| | ATOM | 1291 | N | TYR | A | 164 | 63.140 | 21.031 | 36.958 | 1.00 | 67.44 | 7 |
| | ATOM | 1292 | CA | TYR | A | 164 | 62.968 | 22.396 | 36.466 | 1.00 | 65.48 | 6 |
| | ATOM | 1293 | CB | TYR | A | 164 | 62.085 | 22.422 | 35.221 | 1.00 | 66.46 | 6 |
| | ATOM | 1294 | CG | TYR | A | 164 | 62.709 | 21.754 | 34.029 | 1.00 | 67.56 | 6 |
| 25 | ATOM | 1295 | CD1 | TYR | A | 164 | 62.082 | 20.664 | 33.415 | 1.00 | 68.14 | 6 |
| | ATOM | 1296 | CE1 | TYR | A | 164 | 62.664 | 20.011 | 32.328 | 1.00 | 67.68 | 6 |
| | ATOM | 1297 | CD2 | TYR | A | 164 | 63.942 | 22.185 | 33.527 | 1.00 | 66.99 | 6 |
| | ATOM | 1298 | CE2 | TYR | A | 164 | 64.539 | 21.538 | 32.435 | 1.00 | 69.28 | 6 |
| | ATOM | 1299 | CZ | TYR | A | 164 | 63.892 | 20.449 | 31.837 | 1.00 | 68.44 | 6 |
| 30 | ATOM | 1300 | OH | TYR | A | 164 | 64.456 | 19.823 | 30.737 | 1.00 | 69.00 | 8 |
| | ATOM | 1301 | C | TYR | A | 164 | 62.313 | 23.259 | 37.534 | 1.00 | 64.21 | 6 |
| | ATOM | 1302 | O | TYR | A | 164 | 62.181 | 24.474 | 37.368 | 1.00 | 62.71 | 8 |
| | ATOM | 1303 | N | PHE | A | 165 | 61.899 | 22.626 | 38.627 | 1.00 | 62.72 | 7 |
| | ATOM | 1304 | CA | PHE | A | 165 | 61.241 | 23.343 | 39.705 | 1.00 | 60.48 | 6 |
| 35 | ATOM | 1305 | CB | PHE | A | 165 | 60.738 | 22.364 | 40.758 | 1.00 | 57.99 | 6 |
| | ATOM | 1306 | CG | PHE | A | 165 | 59.676 | 22.936 | 41.641 | 1.00 | 57.14 | 6 |
| | ATOM | 1307 | CD1 | PHE | A | 165 | 58.424 | 23.252 | 41.115 | 1.00 | 55.84 | 6 |
| | ATOM | 1308 | CD2 | PHE | A | 165 | 59.933 | 23.194 | 42.985 | 1.00 | 55.03 | 6 |
| | ATOM | 1309 | CE1 | PHE | A | 165 | 57.439 | 23.818 | 41.902 | 1.00 | 54.80 | 6 |
| 40 | ATOM | 1310 | CE2 | PHE | A | 165 | 58.961 | 23.762 | 43.787 | 1.00 | 57.75 | 6 |
| | ATOM | 1311 | CZ | PHE | A | 165 | 57.699 | 24.079 | 43.242 | 1.00 | 57.78 | 6 |
| | ATOM | 1312 | C | PHE | A | 165 | 62.159 | 24.369 | 40.354 | 1.00 | 60.44 | 6 |
| | ATOM | 1313 | O | PHE | A | 165 | 63.348 | 24.121 | 40.547 | 1.00 | 60.73 | 8 |
| | ATOM | 1314 | N | SER | A | 166 | 61.611 | 25.534 | 40.676 | 1.00 | 60.95 | 7 |
| 45 | ATOM | 1315 | CA | SER | A | 166 | 62.418 | 26.567 | 41.312 | 1.00 | 61.11 | 6 |
| | ATOM | 1316 | CB | SER | A | 166 | 61.638 | 27.874 | 41.457 | 1.00 | 59.76 | 6 |
| | ATOM | 1317 | OG | SER | A | 166 | 62.476 | 28.875 | 42.015 | 1.00 | 59.79 | 8 |
| | ATOM | 1318 | C | SER | A | 166 | 62.809 | 26.068 | 42.694 | 1.00 | 61.38 | 6 |
| | ATOM | 1319 | O | SER | A | 166 | 62.009 | 25.442 | 43.393 | 1.00 | 61.62 | 8 |
| 50 | ATOM | 1320 | N | GLN | A | 167 | 64.038 | 26.359 | 43.089 | 1.00 | 61.82 | 7 |
| | ATOM | 1321 | CA | GLN | A | 167 | 64.525 | 25.931 | 44.393 | 1.00 | 62.17 | 6 |
| | ATOM | 1322 | CB | GLN | A | 167 | 66.052 | 25.797 | 44.351 | 1.00 | 63.58 | 6 |
| | ATOM | 1323 | CG | GLN | A | 167 | 66.745 | 27.065 | 43.861 | 1.00 | 66.42 | 6 |
| | ATOM | 1324 | CD | GLN | A | 167 | 68.204 | 26.851 | 43.514 | 1.00 | 69.06 | 6 |
| 55 | ATOM | 1325 | OE1 | GLN | A | 167 | 69.008 | 26.488 | 44.376 | 1.00 | 70.77 | 8 |
| | ATOM | 1326 | NE2 | GLN | A | 167 | 68.556 | 27.081 | 42.241 | 1.00 | 69.23 | 7 |
| | ATOM | 1327 | C | GLN | A | 167 | 64.119 | 26.927 | 45.476 | 1.00 | 61.22 | 6 |
| | ATOM | 1328 | O | GLN | A | 167 | 64.112 | 26.585 | 46.659 | 1.00 | 61.10 | 8 |
| | ATOM | 1329 | N | TYR | A | 168 | 63.762 | 28.147 | 45.075 | 1.00 | 58.44 | 7 |
| 60 | ATOM | 1330 | CA | TYR | A | 168 | 63.392 | 29.162 | 46.046 | 1.00 | 56.45 | 6 |
| | ATOM | 1331 | CB | TYR | A | 168 | 63.881 | 30.522 | 45.564 | 1.00 | 55.36 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1332 | CG | TYR | A | 168 | 65.335 | 30.469 | 45.158 | 1.00 | 57.58 | 6 |
| | ATOM | 1333 | CD1 | TYR | A | 168 | 65.699 | 30.352 | 43.818 | 1.00 | 57.60 | 6 |
| | ATOM | 1334 | CE1 | TYR | A | 168 | 67.031 | 30.233 | 43.439 | 1.00 | 57.86 | 6 |
| | ATOM | 1335 | CD2 | TYR | A | 168 | 66.349 | 30.467 | 46.115 | 1.00 | 57.43 | 6 |
| 5 | ATOM | 1336 | CE2 | TYR | A | 168 | 67.683 | 30.347 | 45.749 | 1.00 | 58.19 | 6 |
| | ATOM | 1337 | CZ | TYR | A | 168 | 68.017 | 30.228 | 44.410 | 1.00 | 59.25 | 6 |
| | ATOM | 1338 | OH | TYR | A | 168 | 69.337 | 30.086 | 44.042 | 1.00 | 60.91 | 8 |
| | ATOM | 1339 | C | TYR | A | 168 | 61.912 | 29.199 | 46.383 | 1.00 | 56.00 | 6 |
| | ATOM | 1340 | O | TYR | A | 168 | 61.457 | 30.053 | 47.142 | 1.00 | 56.39 | 8 |
| 10 | ATOM | 1341 | N | SER | A | 169 | 61.162 | 28.257 | 45.832 | 1.00 | 55.67 | 7 |
| | ATOM | 1342 | CA | SER | A | 169 | 59.732 | 28.179 | 46.096 | 1.00 | 56.31 | 6 |
| | ATOM | 1343 | CB | SER | A | 169 | 59.082 | 27.123 | 45.197 | 1.00 | 57.76 | 6 |
| | ATOM | 1344 | OG | SER | A | 169 | 57.699 | 26.971 | 45.501 | 1.00 | 55.64 | 8 |
| | ATOM | 1345 | C | SER | A | 169 | 59.478 | 27.804 | 47.544 | 1.00 | 57.69 | 6 |
| 15 | ATOM | 1346 | O | SER | A | 169 | 60.246 | 27.066 | 48.152 | 1.00 | 58.82 | 8 |
| | ATOM | 1347 | N | ARG | A | 170 | 58.385 | 28.302 | 48.096 | 1.00 | 58.68 | 7 |
| | ATOM | 1348 | CA | ARG | A | 170 | 58.043 | 27.993 | 49.472 | 1.00 | 58.62 | 6 |
| | ATOM | 1349 | CB | ARG | A | 170 | 56.907 | 28.901 | 49.956 | 1.00 | 60.14 | 6 |
| | ATOM | 1350 | CG | ARG | A | 170 | 57.371 | 30.123 | 50.727 | 1.00 | 60.43 | 6 |
| 20 | ATOM | 1351 | CD | ARG | A | 170 | 56.401 | 31.291 | 50.589 | 1.00 | 64.30 | 6 |
| | ATOM | 1352 | NE | ARG | A | 170 | 55.020 | 30.998 | 50.989 | 1.00 | 66.31 | 7 |
| | ATOM | 1353 | CZ | ARG | A | 170 | 53.967 | 31.107 | 50.174 | 1.00 | 66.81 | 6 |
| | ATOM | 1354 | NH1 | ARG | A | 170 | 54.129 | 31.489 | 48.915 | 1.00 | 63.97 | 7 |
| | ATOM | 1355 | NH2 | ARG | A | 170 | 52.750 | 30.850 | 50.619 | 1.00 | 67.23 | 7 |
| 25 | ATOM | 1356 | C | ARG | A | 170 | 57.604 | 26.544 | 49.554 | 1.00 | 58.75 | 6 |
| | ATOM | 1357 | O | ARG | A | 170 | 57.516 | 25.975 | 50.642 | 1.00 | 60.59 | 8 |
| | ATOM | 1358 | N | PHE | A | 171 | 57.339 | 25.933 | 48.405 | 1.00 | 57.02 | 7 |
| | ATOM | 1359 | CA | PHE | A | 171 | 56.882 | 24.552 | 48.404 | 1.00 | 56.54 | 6 |
| | ATOM | 1360 | CB | PHE | A | 171 | 55.499 | 24.479 | 47.765 | 1.00 | 55.41 | 6 |
| 30 | ATOM | 1361 | CG | PHE | A | 171 | 54.552 | 25.522 | 48.281 | 1.00 | 55.91 | 6 |
| | ATOM | 1362 | CD1 | PHE | A | 171 | 54.685 | 26.856 | 47.893 | 1.00 | 57.70 | 6 |
| | ATOM | 1363 | CD2 | PHE | A | 171 | 53.560 | 25.190 | 49.203 | 1.00 | 56.28 | 6 |
| | ATOM | 1364 | CE1 | PHE | A | 171 | 53.845 | 27.847 | 48.419 | 1.00 | 58.19 | 6 |
| | ATOM | 1365 | CE2 | PHE | A | 171 | 52.718 | 26.170 | 49.732 | 1.00 | 55.91 | 6 |
| 35 | ATOM | 1366 | CZ | PHE | A | 171 | 52.864 | 27.505 | 49.337 | 1.00 | 57.16 | 6 |
| | ATOM | 1367 | C | PHE | A | 171 | 57.844 | 23.612 | 47.695 | 1.00 | 56.77 | 6 |
| | ATOM | 1368 | O | PHE | A | 171 | 58.841 | 24.045 | 47.113 | 1.00 | 56.03 | 8 |
| | ATOM | 1369 | N | GLU | A | 172 | 57.552 | 22.319 | 47.765 | 1.00 | 56.23 | 7 |
| | ATOM | 1370 | CA | GLU | A | 172 | 58.389 | 21.325 | 47.120 | 1.00 | 58.00 | 6 |
| 40 | ATOM | 1371 | CB | GLU | A | 172 | 59.371 | 20.707 | 48.119 | 1.00 | 60.23 | 6 |
| | ATOM | 1372 | CG | GLU | A | 172 | 58.734 | 19.970 | 49.303 | 1.00 | 64.00 | 6 |
| | ATOM | 1373 | CD | GLU | A | 172 | 59.769 | 19.445 | 50.313 | 1.00 | 66.01 | 6 |
| | ATOM | 1374 | OE1 | GLU | A | 172 | 60.869 | 19.042 | 49.868 | 1.00 | 69.59 | 8 |
| | ATOM | 1375 | OE2 | GLU | A | 172 | 59.487 | 19.421 | 51.541 | 1.00 | 65.33 | 8 |
| 45 | ATOM | 1376 | C | GLU | A | 172 | 57.497 | 20.259 | 46.518 | 1.00 | 59.67 | 6 |
| | ATOM | 1377 | O | GLU | A | 172 | 56.356 | 20.064 | 46.955 | 1.00 | 60.12 | 8 |
| | ATOM | 1378 | N | ILE | A | 173 | 58.006 | 19.579 | 45.496 | 1.00 | 60.16 | 7 |
| | ATOM | 1379 | CA | ILE | A | 173 | 57.224 | 18.545 | 44.827 | 1.00 | 60.67 | 6 |
| | ATOM | 1380 | CB | ILE | A | 173 | 57.413 | 18.587 | 43.291 | 1.00 | 61.87 | 6 |
| 50 | ATOM | 1381 | CG2 | ILE | A | 173 | 56.659 | 17.422 | 42.644 | 1.00 | 62.56 | 6 |
| | ATOM | 1382 | CG1 | ILE | A | 173 | 56.920 | 19.919 | 42.727 | 1.00 | 61.03 | 6 |
| | ATOM | 1383 | CD1 | ILE | A | 173 | 57.165 | 20.062 | 41.244 | 1.00 | 59.49 | 6 |
| | ATOM | 1384 | C | ILE | A | 173 | 57.579 | 17.150 | 45.296 | 1.00 | 59.83 | 6 |
| | ATOM | 1385 | O | ILE | A | 173 | 58.751 | 16.770 | 45.360 | 1.00 | 57.21 | 8 |
| 55 | ATOM | 1386 | N | LEU | A | 174 | 56.554 | 16.381 | 45.616 | 1.00 | 61.63 | 7 |
| | ATOM | 1387 | CA | LEU | A | 174 | 56.786 | 15.022 | 46.056 | 1.00 | 64.20 | 6 |
| | ATOM | 1388 | CB | LEU | A | 174 | 55.687 | 14.592 | 47.024 | 1.00 | 63.47 | 6 |
| | ATOM | 1389 | CG | LEU | A | 174 | 55.461 | 15.601 | 48.149 | 1.00 | 65.34 | 6 |
| | ATOM | 1390 | CD1 | LEU | A | 174 | 54.285 | 15.144 | 49.024 | 1.00 | 66.19 | 6 |
| 60 | ATOM | 1391 | CD2 | LEU | A | 174 | 56.747 | 15.770 | 48.962 | 1.00 | 64.00 | 6 |
| | ATOM | 1392 | C | LEU | A | 174 | 56.783 | 14.147 | 44.806 | 1.00 | 65.92 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1393 | O | LEU | A | 174 | 57.757 | 13.440 | 44.522 | 1.00 | 65.29 | 8 |
| | ATOM | 1394 | N | ASP | A | 175 | 55.702 | 14.233 | 44.036 | 1.00 | 67.33 | 7 |
| | ATOM | 1395 | CA | ASP | A | 175 | 55.583 | 13.436 | 42.827 | 1.00 | 68.45 | 6 |
| | ATOM | 1396 | CB | ASP | A | 175 | 55.227 | 11.993 | 43.223 | 1.00 | 68.56 | 6 |
| 5 | ATOM | 1397 | CG | ASP | A | 175 | 55.161 | 11.038 | 42.032 | 1.00 | 68.23 | 6 |
| | ATOM | 1398 | OD1 | ASP | A | 175 | 56.141 | 10.964 | 41.244 | 1.00 | 67.58 | 8 |
| | ATOM | 1399 | OD2 | ASP | A | 175 | 54.121 | 10.347 | 41.905 | 1.00 | 67.56 | 8 |
| | ATOM | 1400 | C | ASP | A | 175 | 54.542 | 14.023 | 41.872 | 1.00 | 69.02 | 6 |
| | ATOM | 1401 | O | ASP | A | 175 | 53.617 | 14.735 | 42.286 | 1.00 | 69.85 | 8 |
| 10 | ATOM | 1402 | N | VAL | A | 176 | 54.714 | 13.727 | 40.587 | 1.00 | 68.72 | 7 |
| | ATOM | 1403 | CA | VAL | A | 176 | 53.809 | 14.198 | 39.552 | 1.00 | 67.76 | 6 |
| | ATOM | 1404 | CB | VAL | A | 176 | 54.461 | 15.324 | 38.694 | 1.00 | 67.60 | 6 |
| | ATOM | 1405 | CG1 | VAL | A | 176 | 53.533 | 15.721 | 37.542 | 1.00 | 66.09 | 6 |
| | ATOM | 1406 | CG2 | VAL | A | 176 | 54.771 | 16.532 | 39.564 | 1.00 | 65.31 | 6 |
| 15 | ATOM | 1407 | C | VAL | A | 176 | 53.495 | 13.025 | 38.645 | 1.00 | 67.31 | 6 |
| | ATOM | 1408 | O | VAL | A | 176 | 54.399 | 12.308 | 38.230 | 1.00 | 66.10 | 8 |
| | ATOM | 1409 | N | THR | A | 177 | 52.213 | 12.833 | 38.348 | 1.00 | 68.30 | 7 |
| | ATOM | 1410 | CA | THR | A | 177 | 51.781 | 11.763 | 37.463 | 1.00 | 69.37 | 6 |
| | ATOM | 1411 | CB | THR | A | 177 | 51.241 | 10.565 | 38.259 | 1.00 | 69.49 | 6 |
| 20 | ATOM | 1412 | OG1 | THR | A | 177 | 50.218 | 11.007 | 39.160 | 1.00 | 69.60 | 8 |
| | ATOM | 1413 | CG2 | THR | A | 177 | 52.366 | 9.905 | 39.045 | 1.00 | 69.19 | 6 |
| | ATOM | 1414 | C | THR | A | 177 | 50.696 | 12.276 | 36.528 | 1.00 | 70.72 | 6 |
| | ATOM | 1415 | O | THR | A | 177 | 49.879 | 13.119 | 36.917 | 1.00 | 72.04 | 8 |
| | ATOM | 1416 | N | GLN | A | 178 | 50.692 | 11.771 | 35.297 | 1.00 | 71.85 | 7 |
| 25 | ATOM | 1417 | CA | GLN | A | 178 | 49.706 | 12.191 | 34.302 | 1.00 | 73.03 | 6 |
| | ATOM | 1418 | CB | GLN | A | 178 | 50.392 | 12.916 | 33.144 | 1.00 | 75.20 | 6 |
| | ATOM | 1419 | CG | GLN | A | 178 | 51.681 | 13.640 | 33.533 | 1.00 | 78.41 | 6 |
| | ATOM | 1420 | CD | GLN | A | 178 | 52.059 | 14.733 | 32.539 | 1.00 | 79.92 | 6 |
| | ATOM | 1421 | OE1 | GLN | A | 178 | 52.078 | 14.509 | 31.315 | 1.00 | 81.52 | 8 |
| 30 | ATOM | 1422 | NE2 | GLN | A | 178 | 52.370 | 15.924 | 33.061 | 1.00 | 78.36 | 7 |
| | ATOM | 1423 | C | GLN | A | 178 | 49.014 | 10.964 | 33.764 | 1.00 | 72.67 | 6 |
| | ATOM | 1424 | O | GLN | A | 178 | 49.679 | 10.043 | 33.293 | 1.00 | 73.74 | 8 |
| | ATOM | 1425 | N | LYS | A | 179 | 47.686 | 10.947 | 33.827 | 1.00 | 72.17 | 7 |
| | ATOM | 1426 | CA | LYS | A | 179 | 46.916 | 9.807 | 33.337 | 1.00 | 71.53 | 6 |
| 35 | ATOM | 1427 | CB | LYS | A | 179 | 46.327 | 9.038 | 34.519 | 1.00 | 74.09 | 6 |
| | ATOM | 1428 | CG | LYS | A | 179 | 47.352 | 8.781 | 35.644 | 1.00 | 79.46 | 6 |
| | ATOM | 1429 | CD | LYS | A | 179 | 46.703 | 8.189 | 36.905 | 1.00 | 81.06 | 6 |
| | ATOM | 1430 | CE | LYS | A | 179 | 47.635 | 8.300 | 38.119 | 1.00 | 80.77 | 6 |
| | ATOM | 1431 | NZ | LYS | A | 179 | 47.968 | 9.715 | 38.443 | 1.00 | 80.83 | 7 |
| 40 | ATOM | 1432 | C | LYS | A | 179 | 45.795 | 10.316 | 32.470 | 1.00 | 70.00 | 6 |
| | ATOM | 1433 | O | LYS | A | 179 | 44.878 | 10.939 | 32.980 | 1.00 | 73.37 | 8 |
| | ATOM | 1434 | N | LYS | A | 180 | 45.845 | 10.060 | 31.170 | 1.00 | 67.55 | 7 |
| | ATOM | 1435 | CA | LYS | A | 180 | 44.780 | 10.538 | 30.294 | 1.00 | 67.72 | 6 |
| | ATOM | 1436 | CB | LYS | A | 180 | 45.171 | 10.327 | 28.829 | 1.00 | 66.54 | 6 |
| 45 | ATOM | 1437 | CG | LYS | A | 180 | 45.120 | 8.909 | 28.344 | 1.00 | 63.87 | 6 |
| | ATOM | 1438 | CD | LYS | A | 180 | 43.751 | 8.573 | 27.796 | 1.00 | 64.72 | 6 |
| | ATOM | 1439 | CE | LYS | A | 180 | 43.404 | 9.412 | 26.552 | 1.00 | 65.43 | 6 |
| | ATOM | 1440 | NZ | LYS | A | 180 | 44.217 | 9.057 | 25.339 | 1.00 | 65.01 | 7 |
| | ATOM | 1441 | C | LYS | A | 180 | 43.445 | 9.854 | 30.586 | 1.00 | 67.22 | 6 |
| 50 | ATOM | 1442 | O | LYS | A | 180 | 43.373 | 9.021 | 31.471 | 1.00 | 68.12 | 8 |
| | ATOM | 1443 | N | ASN | A | 181 | 42.388 | 10.231 | 29.871 | 1.00 | 67.59 | 7 |
| | ATOM | 1444 | CA | ASN | A | 181 | 41.083 | 9.600 | 30.053 | 1.00 | 68.03 | 6 |
| | ATOM | 1445 | CB | ASN | A | 181 | 40.710 | 9.514 | 31.545 | 1.00 | 69.44 | 6 |
| | ATOM | 1446 | CG | ASN | A | 181 | 40.940 | 10.803 | 32.291 | 1.00 | 68.81 | 6 |
| 55 | ATOM | 1447 | OD1 | ASN | A | 181 | 40.552 | 11.872 | 31.834 | 1.00 | 71.29 | 8 |
| | ATOM | 1448 | ND2 | ASN | A | 181 | 41.556 | 10.706 | 33.463 | 1.00 | 67.88 | 7 |
| | ATOM | 1449 | C | ASN | A | 181 | 39.917 | 10.194 | 29.272 | 1.00 | 67.66 | 6 |
| | ATOM | 1450 | O | ASN | A | 181 | 39.576 | 11.350 | 29.437 | 1.00 | 68.16 | 8 |
| | ATOM | 1451 | N | SER | A | 182 | 39.302 | 9.377 | 28.420 | 1.00 | 68.81 | 7 |
| 60 | ATOM | 1452 | CA | SER | A | 182 | 38.160 | 9.802 | 27.615 | 1.00 | 68.00 | 6 |
| | ATOM | 1453 | CB | SER | A | 182 | 37.861 | 8.745 | 26.553 | 1.00 | 67.42 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|----------|
| 5 | ATOM | 1454 | OG | SER A 182 | 36.905 | 9.223 | 25.626 | 1.00 | 70.87 8 |
| | ATOM | 1455 | C | SER A 182 | 36.953 | 9.974 | 28.541 | 1.00 | 67.36 6 |
| | ATOM | 1456 | O | SER A 182 | 36.915 | 9.385 | 29.617 | 1.00 | 67.61 8 |
| | ATOM | 1457 | N | VAL A 183 | 35.973 | 10.771 | 28.126 | 1.00 | 65.82 7 |
| | ATOM | 1458 | CA | VAL A 183 | 34.790 | 11.017 | 28.950 | 1.00 | 64.66 6 |
| | ATOM | 1459 | CB | VAL A 183 | 35.151 | 11.912 | 30.163 | 1.00 | 63.68 6 |
| | ATOM | 1460 | CG1 | VAL A 183 | 36.153 | 12.956 | 29.748 | 1.00 | 65.08 6 |
| | ATOM | 1461 | CG2 | VAL A 183 | 33.901 | 12.581 | 30.718 | 1.00 | 61.80 6 |
| 10 | ATOM | 1462 | C | VAL A 183 | 33.632 | 11.666 | 28.204 | 1.00 | 64.12 6 |
| | ATOM | 1463 | O | VAL A 183 | 33.828 | 12.597 | 27.440 | 1.00 | 64.83 8 |
| | ATOM | 1464 | N | THR A 184 | 32.422 | 11.170 | 28.432 | 1.00 | 65.00 7 |
| | ATOM | 1465 | CA | THR A 184 | 31.240 | 11.737 | 27.793 | 1.00 | 67.07 6 |
| 15 | ATOM | 1466 | CB | THR A 184 | 30.303 | 10.641 | 27.258 | 1.00 | 64.63 6 |
| | ATOM | 1467 | OG1 | THR A 184 | 30.977 | 9.911 | 26.224 | 1.00 | 61.46 8 |
| | ATOM | 1468 | CG2 | THR A 184 | 29.030 | 11.260 | 26.685 | 1.00 | 67.30 6 |
| | ATOM | 1469 | C | THR A 184 | 30.490 | 12.596 | 28.808 | 1.00 | 69.96 6 |
| 20 | ATOM | 1470 | O | THR A 184 | 30.413 | 12.238 | 29.993 | 1.00 | 71.87 8 |
| | ATOM | 1471 | N | TYR A 185 | 29.961 | 13.735 | 28.362 | 1.00 | 71.00 7 |
| | ATOM | 1472 | CA | TYR A 185 | 29.230 | 14.618 | 29.261 | 1.00 | 72.17 6 |
| | ATOM | 1473 | CB | TYR A 185 | 29.849 | 16.015 | 29.274 | 1.00 | 72.39 6 |
| | ATOM | 1474 | CG | TYR A 185 | 31.335 | 16.005 | 29.525 | 1.00 | 72.53 6 |
| | ATOM | 1475 | CD1 | TYR A 185 | 32.226 | 15.598 | 28.531 | 1.00 | 71.50 6 |
| | ATOM | 1476 | CE1 | TYR A 185 | 33.601 | 15.535 | 28.775 | 1.00 | 70.43 6 |
| | ATOM | 1477 | CD2 | TYR A 185 | 31.854 | 16.358 | 30.776 | 1.00 | 73.42 6 |
| 25 | ATOM | 1478 | CE2 | TYR A 185 | 33.236 | 16.300 | 31.031 | 1.00 | 71.16 6 |
| | ATOM | 1479 | CZ | TYR A 185 | 34.097 | 15.885 | 30.022 | 1.00 | 70.35 6 |
| | ATOM | 1480 | OH | TYR A 185 | 35.448 | 15.811 | 30.254 | 1.00 | 68.69 8 |
| | ATOM | 1481 | C | TYR A 185 | 27.804 | 14.705 | 28.780 | 1.00 | 73.84 6 |
| 30 | ATOM | 1482 | O | TYR A 185 | 27.551 | 14.756 | 27.576 | 1.00 | 73.39 8 |
| | ATOM | 1483 | N | SER A 186 | 26.873 | 14.714 | 29.727 | 1.00 | 76.31 7 |
| | ATOM | 1484 | CA | SER A 186 | 25.455 | 14.794 | 29.403 | 1.00 | 78.23 6 |
| | ATOM | 1485 | CB | SER A 186 | 24.645 | 14.953 | 30.693 | 1.00 | 78.92 6 |
| 35 | ATOM | 1486 | OG | SER A 186 | 25.215 | 15.952 | 31.527 | 1.00 | 77.75 8 |
| | ATOM | 1487 | C | SER A 186 | 25.197 | 15.967 | 28.453 | 1.00 | 78.29 6 |
| | ATOM | 1488 | O | SER A 186 | 24.348 | 15.879 | 27.553 | 1.00 | 79.09 8 |
| | ATOM | 1489 | N | CYS A 187 | 25.949 | 17.047 | 28.653 | 1.00 | 77.81 7 |
| 40 | ATOM | 1490 | CA | CYS A 187 | 25.830 | 18.254 | 27.839 | 1.00 | 78.71 6 |
| | ATOM | 1491 | C | CYS A 187 | 26.144 | 17.978 | 26.407 | 1.00 | 78.06 6 |
| | ATOM | 1492 | O | CYS A 187 | 25.514 | 18.482 | 25.488 | 1.00 | 78.32 8 |
| | ATOM | 1493 | CB | CYS A 187 | 26.858 | 19.320 | 28.252 | 1.00 | 79.52 6 |
| 45 | ATOM | 1494 | SG | CYS A 187 | 28.656 | 18.934 | 27.946 | 1.00 | 82.56 16 |
| | ATOM | 1495 | N | CYS A 188 | 27.147 | 17.144 | 26.244 | 1.00 | 78.96 7 |
| | ATOM | 1496 | CA | CYS A 188 | 27.706 | 16.918 | 24.947 | 1.00 | 78.72 6 |
| | ATOM | 1497 | C | CYS A 188 | 27.817 | 15.468 | 24.454 | 1.00 | 78.19 6 |
| | ATOM | 1498 | O | CYS A 188 | 28.454 | 14.618 | 25.096 | 1.00 | 78.27 8 |
| | ATOM | 1499 | CB | CYS A 188 | 29.070 | 17.610 | 25.006 | 1.00 | 79.96 6 |
| | ATOM | 1500 | SG | CYS A 188 | 29.118 | 19.206 | 25.950 | 1.00 | 80.88 16 |
| | ATOM | 1501 | N | PRO A 189 | 27.211 | 15.186 | 23.281 | 1.00 | 77.44 7 |
| 50 | ATOM | 1502 | CD | PRO A 189 | 26.571 | 16.283 | 22.526 | 1.00 | 77.01 6 |
| | ATOM | 1503 | CA | PRO A 189 | 27.125 | 13.918 | 22.532 | 1.00 | 76.01 6 |
| | ATOM | 1504 | CB | PRO A 189 | 26.756 | 14.378 | 21.129 | 1.00 | 76.94 6 |
| | ATOM | 1505 | CG | PRO A 189 | 25.858 | 15.558 | 21.408 | 1.00 | 77.54 6 |
| 55 | ATOM | 1506 | C | PRO A 189 | 28.355 | 12.991 | 22.512 | 1.00 | 75.22 6 |
| | ATOM | 1507 | O | PRO A 189 | 28.300 | 11.883 | 23.056 | 1.00 | 76.90 8 |
| | ATOM | 1508 | N | GLU A 190 | 29.447 | 13.423 | 21.874 | 1.00 | 72.83 7 |
| | ATOM | 1509 | CA | GLU A 190 | 30.662 | 12.603 | 21.768 | 1.00 | 69.68 6 |
| 60 | ATOM | 1510 | CB | GLU A 190 | 31.535 | 13.102 | 20.629 | 1.00 | 72.91 6 |
| | ATOM | 1511 | CG | GLU A 190 | 30.777 | 13.743 | 19.486 | 1.00 | 75.89 6 |
| | ATOM | 1512 | CD | GLU A 190 | 30.236 | 12.730 | 18.505 | 1.00 | 77.90 6 |
| | ATOM | 1513 | OE1 | GLU A 190 | 30.974 | 11.765 | 18.170 | 1.00 | 78.51 8 |
| | ATOM | 1514 | OE2 | GLU A 190 | 29.080 | 12.909 | 18.058 | 1.00 | 79.55 8 |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| | ATOM | 1515 | C | GLU A 190 | 31.492 | 12.631 | 23.039 | 1.00 | 66.30 | 6 |
| | ATOM | 1516 | O | GLU A 190 | 31.113 | 13.278 | 24.009 | 1.00 | 65.23 | 8 |
| | ATOM | 1517 | N | ALA A 191 | 32.633 | 11.941 | 23.020 | 1.00 | 63.17 | 7 |
| | ATOM | 1518 | CA | ALA A 191 | 33.524 | 11.891 | 24.182 | 1.00 | 61.94 | 6 |
| 5 | ATOM | 1519 | CB | ALA A 191 | 34.102 | 10.493 | 24.341 | 1.00 | 60.63 | 6 |
| | ATOM | 1520 | C | ALA A 191 | 34.666 | 12.904 | 24.055 | 1.00 | 61.30 | 6 |
| | ATOM | 1521 | O | ALA A 191 | 35.148 | 13.165 | 22.950 | 1.00 | 62.21 | 8 |
| | ATOM | 1522 | N | TYR A 192 | 35.105 | 13.468 | 25.179 | 1.00 | 58.30 | 7 |
| | ATOM | 1523 | CA | TYR A 192 | 36.188 | 14.438 | 25.159 | 1.00 | 56.19 | 6 |
| 10 | ATOM | 1524 | CB | TYR A 192 | 35.695 | 15.807 | 25.633 | 1.00 | 55.84 | 6 |
| | ATOM | 1525 | CG | TYR A 192 | 34.779 | 16.487 | 24.649 | 1.00 | 56.15 | 6 |
| | ATOM | 1526 | CD1 | TYR A 192 | 33.409 | 16.226 | 24.642 | 1.00 | 56.04 | 6 |
| | ATOM | 1527 | CE1 | TYR A 192 | 32.571 | 16.794 | 23.683 | 1.00 | 57.88 | 6 |
| | ATOM | 1528 | CD2 | TYR A 192 | 35.291 | 17.341 | 23.675 | 1.00 | 56.39 | 6 |
| 15 | ATOM | 1529 | CE2 | TYR A 192 | 34.467 | 17.915 | 22.715 | 1.00 | 57.19 | 6 |
| | ATOM | 1530 | CZ | TYR A 192 | 33.108 | 17.637 | 22.722 | 1.00 | 58.29 | 6 |
| | ATOM | 1531 | OH | TYR A 192 | 32.295 | 18.200 | 21.769 | 1.00 | 58.06 | 8 |
| | ATOM | 1532 | C | TYR A 192 | 37.389 | 14.013 | 25.984 | 1.00 | 56.62 | 6 |
| | ATOM | 1533 | O | TYR A 192 | 37.375 | 14.090 | 27.217 | 1.00 | 57.67 | 8 |
| 20 | ATOM | 1534 | N | GLU A 193 | 38.436 | 13.571 | 25.291 | 1.00 | 57.15 | 7 |
| | ATOM | 1535 | CA | GLU A 193 | 39.676 | 13.124 | 25.935 | 1.00 | 58.07 | 6 |
| | ATOM | 1536 | CB | GLU A 193 | 40.651 | 12.523 | 24.901 | 1.00 | 56.63 | 6 |
| | ATOM | 1537 | CG | GLU A 193 | 40.143 | 11.269 | 24.209 | 1.00 | 55.92 | 6 |
| | ATOM | 1538 | CD | GLU A 193 | 41.171 | 10.636 | 23.307 | 1.00 | 56.05 | 6 |
| 25 | ATOM | 1539 | OE1 | GLU A 193 | 42.339 | 10.509 | 23.743 | 1.00 | 56.33 | 8 |
| | ATOM | 1540 | OE2 | GLU A 193 | 40.808 | 10.250 | 22.171 | 1.00 | 57.19 | 8 |
| | ATOM | 1541 | C | GLU A 193 | 40.363 | 14.278 | 26.655 | 1.00 | 58.09 | 6 |
| | ATOM | 1542 | O | GLU A 193 | 40.221 | 15.440 | 26.261 | 1.00 | 59.15 | 8 |
| | ATOM | 1543 | N | ASP A 194 | 41.098 | 13.948 | 27.712 | 1.00 | 57.73 | 7 |
| 30 | ATOM | 1544 | CA | ASP A 194 | 41.816 | 14.941 | 28.486 | 1.00 | 56.31 | 6 |
| | ATOM | 1545 | CB | ASP A 194 | 40.856 | 15.738 | 29.386 | 1.00 | 57.85 | 6 |
| | ATOM | 1546 | CG | ASP A 194 | 40.339 | 14.930 | 30.578 | 1.00 | 59.72 | 6 |
| | ATOM | 1547 | OD1 | ASP A 194 | 39.120 | 14.610 | 30.592 | 1.00 | 55.87 | 8 |
| | ATOM | 1548 | OD2 | ASP A 194 | 41.154 | 14.628 | 31.494 | 1.00 | 58.60 | 8 |
| 35 | ATOM | 1549 | C | ASP A 194 | 42.881 | 14.276 | 29.333 | 1.00 | 55.87 | 6 |
| | ATOM | 1550 | O | ASP A 194 | 42.746 | 13.121 | 29.714 | 1.00 | 56.72 | 8 |
| | ATOM | 1551 | N | VAL A 195 | 43.948 | 15.014 | 29.611 | 1.00 | 55.00 | 7 |
| | ATOM | 1552 | CA | VAL A 195 | 45.039 | 14.520 | 30.431 | 1.00 | 55.58 | 6 |
| | ATOM | 1553 | CB | VAL A 195 | 46.397 | 14.961 | 29.876 | 1.00 | 54.15 | 6 |
| 40 | ATOM | 1554 | CG1 | VAL A 195 | 47.508 | 14.610 | 30.860 | 1.00 | 52.00 | 6 |
| | ATOM | 1555 | CG2 | VAL A 195 | 46.643 | 14.292 | 28.544 | 1.00 | 53.83 | 6 |
| | ATOM | 1556 | C | VAL A 195 | 44.900 | 15.082 | 31.832 | 1.00 | 57.46 | 6 |
| | ATOM | 1557 | O | VAL A 195 | 44.809 | 16.294 | 32.011 | 1.00 | 57.93 | 8 |
| | ATOM | 1558 | N | GLU A 196 | 44.886 | 14.206 | 32.828 | 1.00 | 58.46 | 7 |
| 45 | ATOM | 1559 | CA | GLU A 196 | 44.767 | 14.654 | 34.204 | 1.00 | 58.24 | 6 |
| | ATOM | 1560 | CB | GLU A 196 | 43.805 | 13.758 | 34.966 | 1.00 | 59.77 | 6 |
| | ATOM | 1561 | CG | GLU A 196 | 43.556 | 14.199 | 36.385 | 1.00 | 63.27 | 6 |
| | ATOM | 1562 | CD | GLU A 196 | 42.624 | 13.256 | 37.114 | 1.00 | 64.52 | 6 |
| | ATOM | 1563 | OE1 | GLU A 196 | 41.485 | 13.063 | 36.646 | 1.00 | 63.73 | 8 |
| 50 | ATOM | 1564 | OE2 | GLU A 196 | 43.035 | 12.705 | 38.155 | 1.00 | 68.58 | 8 |
| | ATOM | 1565 | C | GLU A 196 | 46.142 | 14.590 | 34.828 | 1.00 | 57.57 | 6 |
| | ATOM | 1566 | O | GLU A 196 | 46.775 | 13.538 | 34.841 | 1.00 | 59.03 | 8 |
| | ATOM | 1567 | N | VAL A 197 | 46.618 | 15.723 | 35.322 | 1.00 | 55.78 | 7 |
| | ATOM | 1568 | CA | VAL A 197 | 47.929 | 15.766 | 35.943 | 1.00 | 55.65 | 6 |
| 55 | ATOM | 1569 | CB | VAL A 197 | 48.781 | 16.937 | 35.386 | 1.00 | 55.24 | 6 |
| | ATOM | 1570 | CG1 | VAL A 197 | 50.142 | 16.962 | 36.050 | 1.00 | 51.21 | 6 |
| | ATOM | 1571 | CG2 | VAL A 197 | 48.929 | 16.800 | 33.877 | 1.00 | 53.65 | 6 |
| | ATOM | 1572 | C | VAL A 197 | 47.716 | 15.955 | 37.431 | 1.00 | 57.58 | 6 |
| | ATOM | 1573 | O | VAL A 197 | 46.963 | 16.843 | 37.850 | 1.00 | 57.66 | 8 |
| 60 | ATOM | 1574 | N | SER A 198 | 48.355 | 15.102 | 38.231 | 1.00 | 58.29 | 7 |
| | ATOM | 1575 | CA | SER A 198 | 48.229 | 15.194 | 39.677 | 1.00 | 57.91 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1576 | CB | SER A 198 | 47.951 | 13.822 | 40.275 | 1.00 | 56.54 | 6 |
| | ATOM | 1577 | OG | SER A 198 | 46.654 | 13.401 | 39.908 | 1.00 | 61.46 | 8 |
| | ATOM | 1578 | C | SER A 198 | 49.501 | 15.765 | 40.257 | 1.00 | 58.27 | 6 |
| | ATOM | 1579 | O | SER A 198 | 50.585 | 15.202 | 40.089 | 1.00 | 58.63 | 8 |
| | ATOM | 1580 | N | LEU A 199 | 49.366 | 16.901 | 40.929 | 1.00 | 58.53 | 7 |
| 10 | ATOM | 1581 | CA | LEU A 199 | 50.521 | 17.538 | 41.531 | 1.00 | 60.77 | 6 |
| | ATOM | 1582 | CB | LEU A 199 | 50.519 | 19.046 | 41.274 | 1.00 | 60.73 | 6 |
| | ATOM | 1583 | CG | LEU A 199 | 51.591 | 19.833 | 42.032 | 1.00 | 59.19 | 6 |
| | ATOM | 1584 | CD1 | LEU A 199 | 52.982 | 19.400 | 41.599 | 1.00 | 57.61 | 6 |
| | ATOM | 1585 | CD2 | LEU A 199 | 51.390 | 21.311 | 41.776 | 1.00 | 60.66 | 6 |
| 15 | ATOM | 1586 | C | LEU A 199 | 50.524 | 17.293 | 43.022 | 1.00 | 61.78 | 6 |
| | ATOM | 1587 | O | LEU A 199 | 49.739 | 17.895 | 43.765 | 1.00 | 62.31 | 8 |
| | ATOM | 1588 | N | ASN A 200 | 51.397 | 16.389 | 43.457 | 1.00 | 61.40 | 7 |
| | ATOM | 1589 | CA | ASN A 200 | 51.519 | 16.092 | 44.866 | 1.00 | 58.00 | 6 |
| | ATOM | 1590 | CB | ASN A 200 | 51.763 | 14.607 | 45.088 | 1.00 | 60.46 | 6 |
| 20 | ATOM | 1591 | CG | ASN A 200 | 51.926 | 14.267 | 46.553 | 1.00 | 61.99 | 6 |
| | ATOM | 1592 | OD1 | ASN A 200 | 51.158 | 14.735 | 47.391 | 1.00 | 63.14 | 8 |
| | ATOM | 1593 | ND2 | ASN A 200 | 52.928 | 13.447 | 46.871 | 1.00 | 63.54 | 7 |
| | ATOM | 1594 | C | ASN A 200 | 52.708 | 16.906 | 45.345 | 1.00 | 56.52 | 6 |
| | ATOM | 1595 | O | ASN A 200 | 53.859 | 16.664 | 44.957 | 1.00 | 55.31 | 8 |
| 25 | ATOM | 1596 | N | PHE A 201 | 52.406 | 17.901 | 46.166 | 1.00 | 55.49 | 7 |
| | ATOM | 1597 | CA | PHE A 201 | 53.416 | 18.790 | 46.707 | 1.00 | 54.84 | 6 |
| | ATOM | 1598 | CB | PHE A 201 | 53.450 | 20.082 | 45.908 | 1.00 | 50.77 | 6 |
| | ATOM | 1599 | CG | PHE A 201 | 52.237 | 20.940 | 46.112 | 1.00 | 47.21 | 6 |
| | ATOM | 1600 | CD1 | PHE A 201 | 52.337 | 22.161 | 46.765 | 1.00 | 46.20 | 6 |
| 30 | ATOM | 1601 | CD2 | PHE A 201 | 50.985 | 20.513 | 45.678 | 1.00 | 46.31 | 6 |
| | ATOM | 1602 | CE1 | PHE A 201 | 51.205 | 22.942 | 46.984 | 1.00 | 45.24 | 6 |
| | ATOM | 1603 | CE2 | PHE A 201 | 49.849 | 21.291 | 45.896 | 1.00 | 43.16 | 6 |
| | ATOM | 1604 | CZ | PHE A 201 | 49.962 | 22.504 | 46.549 | 1.00 | 42.59 | 6 |
| | ATOM | 1605 | C | PHE A 201 | 53.035 | 19.112 | 48.142 | 1.00 | 56.47 | 6 |
| 35 | ATOM | 1606 | O | PHE A 201 | 51.956 | 18.748 | 48.610 | 1.00 | 54.75 | 8 |
| | ATOM | 1607 | N | ARG A 202 | 53.927 | 19.811 | 48.829 | 1.00 | 58.72 | 7 |
| | ATOM | 1608 | CA | ARG A 202 | 53.693 | 20.207 | 50.207 | 1.00 | 61.75 | 6 |
| | ATOM | 1609 | CB | ARG A 202 | 54.052 | 19.063 | 51.136 | 1.00 | 63.76 | 6 |
| | ATOM | 1610 | CG | ARG A 202 | 55.544 | 18.822 | 51.130 | 1.00 | 65.86 | 6 |
| 40 | ATOM | 1611 | CD | ARG A 202 | 55.938 | 17.640 | 51.962 | 1.00 | 68.52 | 6 |
| | ATOM | 1612 | NE | ARG A 202 | 57.383 | 17.466 | 51.916 | 1.00 | 69.87 | 7 |
| | ATOM | 1613 | CZ | ARG A 202 | 58.013 | 16.409 | 52.405 | 1.00 | 70.56 | 6 |
| | ATOM | 1614 | NH1 | ARG A 202 | 57.308 | 15.433 | 52.977 | 1.00 | 71.39 | 7 |
| | ATOM | 1615 | NH2 | ARG A 202 | 59.340 | 16.332 | 52.315 | 1.00 | 70.56 | 7 |
| 45 | ATOM | 1616 | C | ARG A 202 | 54.579 | 21.406 | 50.556 | 1.00 | 62.74 | 6 |
| | ATOM | 1617 | O | ARG A 202 | 55.588 | 21.675 | 49.890 | 1.00 | 62.41 | 8 |
| | ATOM | 1618 | N | LYS A 203 | 54.200 | 22.121 | 51.606 | 1.00 | 63.53 | 7 |
| | ATOM | 1619 | CA | LYS A 203 | 54.983 | 23.256 | 52.044 | 1.00 | 64.89 | 6 |
| | ATOM | 1620 | CB | LYS A 203 | 54.271 | 23.993 | 53.169 | 1.00 | 65.59 | 6 |
| 50 | ATOM | 1621 | CG | LYS A 203 | 55.067 | 25.149 | 53.740 | 1.00 | 66.14 | 6 |
| | ATOM | 1622 | CD | LYS A 203 | 54.348 | 25.777 | 54.911 | 1.00 | 65.85 | 6 |
| | ATOM | 1623 | CE | LYS A 203 | 55.145 | 26.939 | 55.473 | 1.00 | 67.46 | 6 |
| | ATOM | 1624 | NZ | LYS A 203 | 55.259 | 28.073 | 54.500 | 1.00 | 68.09 | 7 |
| | ATOM | 1625 | C | LYS A 203 | 56.264 | 22.665 | 52.563 | 1.00 | 65.93 | 6 |
| 55 | ATOM | 1626 | O | LYS A 203 | 56.250 | 21.585 | 53.157 | 1.00 | 66.11 | 8 |
| | ATOM | 1627 | N | LYS A 204 | 57.372 | 23.351 | 52.313 | 1.00 | 69.05 | 7 |
| | ATOM | 1628 | CA | LYS A 204 | 58.659 | 22.863 | 52.767 | 1.00 | 71.58 | 6 |
| | ATOM | 1629 | CB | LYS A 204 | 59.758 | 23.834 | 52.358 | 1.00 | 69.66 | 6 |
| | ATOM | 1630 | CG | LYS A 204 | 59.862 | 23.906 | 50.839 | 1.00 | 69.91 | 6 |
| 60 | ATOM | 1631 | CD | LYS A 204 | 61.113 | 24.609 | 50.336 | 1.00 | 71.48 | 6 |
| | ATOM | 1632 | CE | LYS A 204 | 61.195 | 24.491 | 48.809 | 1.00 | 73.18 | 6 |
| | ATOM | 1633 | NZ | LYS A 204 | 62.324 | 25.234 | 48.189 | 1.00 | 72.99 | 7 |
| | ATOM | 1634 | C | LYS A 204 | 58.544 | 22.745 | 54.264 | 1.00 | 74.56 | 6 |
| | ATOM | 1635 | O | LYS A 204 | 57.769 | 23.493 | 54.873 | 1.00 | 77.21 | 8 |
| | ATOM | 1636 | N | GLY A 205 | 59.262 | 21.782 | 54.850 | 1.00 | 75.75 | 7 |

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|----|------|------|-----|-----------|--------|--------|--------|------|---------|
| 5 | ATOM | 1637 | CA | GLY A 205 | 59.215 | 21.592 | 56.296 | 1.00 | 75.55 6 |
| | ATOM | 1638 | C | GLY A 205 | 60.125 | 22.564 | 57.029 | 1.00 | 76.09 6 |
| | ATOM | 1639 | OT1 | GLY A 205 | 60.824 | 23.350 | 56.348 | 1.00 | 77.07 8 |
| | ATOM | 1640 | OT2 | GLY A 205 | 60.151 | 22.545 | 58.278 | 1.00 | 75.36 8 |
| | ATOM | 1641 | CB | PHE B 1 | 33.107 | 19.922 | 1.832 | 1.00 | 57.02 6 |
| 10 | ATOM | 1642 | CG | PHE B 1 | 32.174 | 20.672 | 0.888 | 1.00 | 58.55 6 |
| | ATOM | 1643 | CD1 | PHE B 1 | 32.670 | 21.495 | -0.120 | 1.00 | 59.39 6 |
| | ATOM | 1644 | CD2 | PHE B 1 | 30.784 | 20.612 | 1.079 | 1.00 | 58.84 6 |
| | ATOM | 1645 | CE1 | PHE B 1 | 31.795 | 22.248 | -0.919 | 1.00 | 59.92 6 |
| | ATOM | 1646 | CE2 | PHE B 1 | 29.905 | 21.357 | 0.292 | 1.00 | 56.97 6 |
| 15 | ATOM | 1647 | CZ | PHE B 1 | 30.410 | 22.176 | -0.707 | 1.00 | 58.52 6 |
| | ATOM | 1648 | C | PHE B 1 | 35.200 | 18.747 | 2.262 | 1.00 | 56.22 6 |
| | ATOM | 1649 | O | PHE B 1 | 34.732 | 18.314 | 3.311 | 1.00 | 58.27 8 |
| | ATOM | 1650 | N | PHE B 1 | 33.748 | 17.916 | 0.462 | 1.00 | 54.28 7 |
| | ATOM | 1651 | CA | PHE B 1 | 34.250 | 19.143 | 1.152 | 1.00 | 55.90 6 |
| 20 | ATOM | 1652 | N | ASP B 2 | 36.512 | 18.877 | 2.083 | 1.00 | 55.99 7 |
| | ATOM | 1653 | CA | ASP B 2 | 37.383 | 18.526 | 3.204 | 1.00 | 56.44 6 |
| | ATOM | 1654 | CB | ASP B 2 | 38.876 | 18.485 | 2.792 | 1.00 | 59.88 6 |
| | ATOM | 1655 | CG | ASP B 2 | 39.364 | 19.782 | 2.139 | 1.00 | 65.04 6 |
| | ATOM | 1656 | OD1 | ASP B 2 | 40.076 | 19.729 | 1.091 | 1.00 | 67.12 8 |
| 25 | ATOM | 1657 | OD2 | ASP B 2 | 39.042 | 20.860 | 2.684 | 1.00 | 68.18 8 |
| | ATOM | 1658 | C | ASP B 2 | 37.096 | 19.582 | 4.280 | 1.00 | 55.70 6 |
| | ATOM | 1659 | O | ASP B 2 | 36.331 | 20.507 | 4.047 | 1.00 | 54.61 8 |
| | ATOM | 1660 | N | ARG B 3 | 37.682 | 19.443 | 5.458 | 1.00 | 55.52 7 |
| | ATOM | 1661 | CA | ARG B 3 | 37.441 | 20.380 | 6.556 | 1.00 | 53.72 6 |
| 30 | ATOM | 1662 | CB | ARG B 3 | 38.114 | 19.838 | 7.806 | 1.00 | 56.23 6 |
| | ATOM | 1663 | CG | ARG B 3 | 37.541 | 20.323 | 9.094 | 1.00 | 55.76 6 |
| | ATOM | 1664 | CD | ARG B 3 | 37.772 | 19.269 | 10.139 | 1.00 | 55.83 6 |
| | ATOM | 1665 | NE | ARG B 3 | 36.531 | 18.930 | 10.818 | 1.00 | 56.35 7 |
| | ATOM | 1666 | CZ | ARG B 3 | 36.233 | 17.708 | 11.220 | 1.00 | 56.91 6 |
| 35 | ATOM | 1667 | NH1 | ARG B 3 | 37.095 | 16.729 | 10.994 | 1.00 | 56.22 7 |
| | ATOM | 1668 | NH2 | ARG B 3 | 35.090 | 17.468 | 11.849 | 1.00 | 57.84 7 |
| | ATOM | 1669 | C | ARG B 3 | 37.909 | 21.822 | 6.295 | 1.00 | 53.67 6 |
| | ATOM | 1670 | O | ARG B 3 | 37.395 | 22.772 | 6.888 | 1.00 | 53.80 8 |
| | ATOM | 1671 | N | ALA B 4 | 38.896 | 21.969 | 5.420 | 1.00 | 52.29 7 |
| 40 | ATOM | 1672 | CA | ALA B 4 | 39.443 | 23.255 | 5.025 | 1.00 | 50.06 6 |
| | ATOM | 1673 | CB | ALA B 4 | 40.743 | 23.036 | 4.275 | 1.00 | 48.42 6 |
| | ATOM | 1674 | C | ALA B 4 | 38.442 | 23.978 | 4.131 | 1.00 | 49.06 6 |
| | ATOM | 1675 | O | ALA B 4 | 38.225 | 25.179 | 4.270 | 1.00 | 47.12 8 |
| | ATOM | 1676 | N | ASP B 5 | 37.837 | 23.233 | 3.211 | 1.00 | 49.07 7 |
| 45 | ATOM | 1677 | CA | ASP B 5 | 36.869 | 23.801 | 2.288 | 1.00 | 51.75 6 |
| | ATOM | 1678 | CB | ASP B 5 | 36.345 | 22.748 | 1.299 | 1.00 | 55.02 6 |
| | ATOM | 1679 | CG | ASP B 5 | 37.454 | 22.084 | 0.491 | 1.00 | 60.18 6 |
| | ATOM | 1680 | OD1 | ASP B 5 | 38.347 | 22.794 | -0.039 | 1.00 | 63.04 8 |
| | ATOM | 1681 | OD2 | ASP B 5 | 37.430 | 20.839 | 0.374 | 1.00 | 61.10 8 |
| 50 | ATOM | 1682 | C | ASP B 5 | 35.699 | 24.381 | 3.051 | 1.00 | 51.17 6 |
| | ATOM | 1683 | O | ASP B 5 | 35.179 | 25.428 | 2.670 | 1.00 | 51.32 8 |
| | ATOM | 1684 | N | ILE B 6 | 35.292 | 23.713 | 4.130 | 1.00 | 49.73 7 |
| | ATOM | 1685 | CA | ILE B 6 | 34.164 | 24.178 | 4.926 | 1.00 | 50.09 6 |
| | ATOM | 1686 | CB | ILE B 6 | 33.723 | 23.128 | 5.950 | 1.00 | 51.11 6 |
| 55 | ATOM | 1687 | CG2 | ILE B 6 | 32.472 | 23.610 | 6.678 | 1.00 | 48.60 6 |
| | ATOM | 1688 | CG1 | ILE B 6 | 33.434 | 21.809 | 5.232 | 1.00 | 53.13 6 |
| | ATOM | 1689 | CD1 | ILE B 6 | 32.881 | 20.712 | 6.121 | 1.00 | 55.06 6 |
| | ATOM | 1690 | C | ILE B 6 | 34.448 | 25.480 | 5.653 | 1.00 | 49.98 6 |
| | ATOM | 1691 | O | ILE B 6 | 33.700 | 26.450 | 5.518 | 1.00 | 51.60 8 |
| 60 | ATOM | 1692 | N | LEU B 7 | 35.524 | 25.504 | 6.426 | 1.00 | 49.48 7 |
| | ATOM | 1693 | CA | LEU B 7 | 35.908 | 26.705 | 7.160 | 1.00 | 48.15 6 |
| | ATOM | 1694 | CB | LEU B 7 | 37.157 | 26.424 | 7.995 | 1.00 | 45.60 6 |
| | ATOM | 1695 | CG | LEU B 7 | 36.916 | 25.427 | 9.126 | 1.00 | 45.98 6 |
| | ATOM | 1696 | CD1 | LEU B 7 | 38.221 | 24.935 | 9.696 | 1.00 | 46.59 6 |
| | ATOM | 1697 | CD2 | LEU B 7 | 36.081 | 26.086 | 10.191 | 1.00 | 44.50 6 |

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|----|------|------|-----|-------|------|--------|--------|--------|--------------|
| 5 | ATOM | 1698 | C | LEU B | 7 | 36.167 | 27.850 | 6.195 | 1.00 47.43 6 |
| | ATOM | 1699 | O | LEU B | 7 | 35.797 | 28.986 | 6.447 | 1.00 46.94 8 |
| | ATOM | 1700 | N | TYR B | 8 | 36.799 | 27.529 | 5.080 | 1.00 49.45 7 |
| | ATOM | 1701 | CA | TYR B | 8 | 37.105 | 28.507 | 4.051 | 1.00 52.16 6 |
| | ATOM | 1702 | CB | TYR B | 8 | 37.800 | 27.821 | 2.877 | 1.00 54.75 6 |
| | ATOM | 1703 | CG | TYR B | 8 | 38.090 | 28.758 | 1.737 | 1.00 56.10 6 |
| | ATOM | 1704 | CD1 | TYR B | 8 | 39.088 | 29.720 | 1.839 | 1.00 56.48 6 |
| | ATOM | 1705 | CE1 | TYR B | 8 | 39.344 | 30.605 | 0.794 | 1.00 57.35 6 |
| 10 | ATOM | 1706 | CD2 | TYR B | 8 | 37.348 | 28.701 | 0.564 | 1.00 57.26 6 |
| | ATOM | 1707 | CE2 | TYR B | 8 | 37.592 | 29.581 | -0.484 | 1.00 57.99 6 |
| | ATOM | 1708 | CZ | TYR B | 8 | 38.590 | 30.528 | -0.364 | 1.00 57.33 6 |
| | ATOM | 1709 | OH | TYR B | 8 | 38.819 | 31.385 | -1.408 | 1.00 58.94 8 |
| 15 | ATOM | 1710 | C | TYR B | 8 | 35.858 | 29.234 | 3.537 | 1.00 52.55 6 |
| | ATOM | 1711 | O | TYR B | 8 | 35.867 | 30.460 | 3.387 | 1.00 52.22 8 |
| | ATOM | 1712 | N | ASN B | 9 | 34.796 | 28.482 | 3.249 | 1.00 52.51 7 |
| | ATOM | 1713 | CA | ASN B | 9 | 33.566 | 29.086 | 2.752 | 1.00 54.09 6 |
| | ATOM | 1714 | CB | ASN B | 9 | 32.539 | 28.021 | 2.376 | 1.00 56.72 6 |
| | ATOM | 1715 | CG | ASN B | 9 | 32.963 | 27.203 | 1.163 | 1.00 60.46 6 |
| | ATOM | 1716 | OD1 | ASN B | 9 | 33.966 | 27.509 | 0.512 | 1.00 61.72 8 |
| | ATOM | 1717 | ND2 | ASN B | 9 | 32.198 | 26.159 | 0.852 | 1.00 61.67 7 |
| 20 | ATOM | 1718 | C | ASN B | 9 | 32.980 | 30.007 | 3.794 | 1.00 54.24 6 |
| | ATOM | 1719 | O | ASN B | 9 | 32.680 | 31.160 | 3.506 | 1.00 54.66 8 |
| | ATOM | 1720 | N | ILE B | 10 | 32.829 | 29.503 | 5.013 | 1.00 54.21 7 |
| | ATOM | 1721 | CA | ILE B | 10 | 32.282 | 30.310 | 6.104 | 1.00 53.77 6 |
| | ATOM | 1722 | CB | ILE B | 10 | 32.303 | 29.543 | 7.429 | 1.00 52.00 6 |
| | ATOM | 1723 | CG2 | ILE B | 10 | 31.860 | 30.451 | 8.552 | 1.00 50.79 6 |
| | ATOM | 1724 | CG1 | ILE B | 10 | 31.389 | 28.323 | 7.339 | 1.00 50.43 6 |
| | ATOM | 1725 | CD1 | ILE B | 10 | 31.531 | 27.371 | 8.498 | 1.00 47.56 6 |
| 30 | ATOM | 1726 | C | ILE B | 10 | 33.085 | 31.592 | 6.284 | 1.00 55.12 6 |
| | ATOM | 1727 | O | ILE B | 10 | 32.531 | 32.663 | 6.458 | 1.00 56.17 8 |
| | ATOM | 1728 | N | ARG B | 11 | 34.400 | 31.464 | 6.243 | 1.00 56.91 7 |
| | ATOM | 1729 | CA | ARG B | 11 | 35.297 | 32.595 | 6.386 | 1.00 58.48 6 |
| | ATOM | 1730 | CB | ARG B | 11 | 36.739 | 32.110 | 6.243 | 1.00 63.85 6 |
| | ATOM | 1731 | CG | ARG B | 11 | 37.799 | 33.170 | 6.434 | 1.00 68.86 6 |
| | ATOM | 1732 | CD | ARG B | 11 | 37.917 | 33.493 | 7.917 | 1.00 77.74 6 |
| | ATOM | 1733 | NE | ARG B | 11 | 39.211 | 34.078 | 8.264 | 1.00 85.52 7 |
| 35 | ATOM | 1734 | CZ | ARG B | 11 | 40.384 | 33.635 | 7.807 | 1.00 88.55 6 |
| | ATOM | 1735 | NH1 | ARG B | 11 | 40.424 | 32.589 | 6.970 | 1.00 90.95 7 |
| | ATOM | 1736 | NH2 | ARG B | 11 | 41.518 | 34.239 | 8.178 | 1.00 87.63 7 |
| | ATOM | 1737 | C | ARG B | 11 | 35.030 | 33.639 | 5.306 | 1.00 58.49 6 |
| | ATOM | 1738 | O | ARG B | 11 | 34.905 | 34.825 | 5.584 | 1.00 57.34 8 |
| | ATOM | 1739 | N | GLN B | 12 | 34.933 | 33.175 | 4.066 | 1.00 58.50 7 |
| | ATOM | 1740 | CA | GLN B | 12 | 34.748 | 34.055 | 2.927 | 1.00 57.77 6 |
| | ATOM | 1741 | CB | GLN B | 12 | 35.147 | 33.329 | 1.653 | 1.00 58.35 6 |
| 45 | ATOM | 1742 | CG | GLN B | 12 | 36.124 | 34.100 | 0.814 | 1.00 62.22 6 |
| | ATOM | 1743 | CD | GLN B | 12 | 37.514 | 33.973 | 1.351 | 1.00 64.08 6 |
| | ATOM | 1744 | OE1 | GLN B | 12 | 38.011 | 32.862 | 1.501 | 1.00 68.35 8 |
| | ATOM | 1745 | NE2 | GLN B | 12 | 38.156 | 35.098 | 1.653 | 1.00 63.78 7 |
| | ATOM | 1746 | C | GLN B | 12 | 33.366 | 34.633 | 2.720 | 1.00 57.86 6 |
| | ATOM | 1747 | O | GLN B | 12 | 33.219 | 35.657 | 2.059 | 1.00 59.62 8 |
| | ATOM | 1748 | N | THR B | 13 | 32.345 | 33.994 | 3.266 | 1.00 57.21 7 |
| | ATOM | 1749 | CA | THR B | 13 | 30.987 | 34.479 | 3.054 | 1.00 56.88 6 |
| 55 | ATOM | 1750 | CB | THR B | 13 | 30.101 | 33.373 | 2.468 | 1.00 54.90 6 |
| | ATOM | 1751 | OG1 | THR B | 13 | 30.100 | 32.247 | 3.350 | 1.00 55.07 8 |
| | ATOM | 1752 | CG2 | THR B | 13 | 30.612 | 32.946 | 1.104 | 1.00 56.83 6 |
| | ATOM | 1753 | C | THR B | 13 | 30.295 | 35.009 | 4.298 | 1.00 58.52 6 |
| | ATOM | 1754 | O | THR B | 13 | 29.275 | 35.698 | 4.206 | 1.00 57.64 8 |
| | ATOM | 1755 | N | SER B | 14 | 30.848 | 34.691 | 5.462 | 1.00 60.24 7 |
| | ATOM | 1756 | CA | SER B | 14 | 30.247 | 35.117 | 6.715 | 1.00 60.31 6 |
| | ATOM | 1757 | CB | SER B | 14 | 30.884 | 34.369 | 7.878 | 1.00 60.50 6 |
| 60 | ATOM | 1758 | OG | SER B | 14 | 30.086 | 34.485 | 9.034 | 1.00 63.18 8 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 1759 | C | SER | B | 14 | 30.343 | 36.619 | 6.949 | 1.00 | 59.80 | 6 |
| | ATOM | 1760 | O | SER | B | 14 | 31.247 | 37.293 | 6.443 | 1.00 | 60.23 | 8 |
| | ATOM | 1761 | N | ARG | B | 15 | 29.382 | 37.134 | 7.710 | 1.00 | 58.15 | 7 |
| | ATOM | 1762 | CA | ARG | B | 15 | 29.322 | 38.549 | 8.040 | 1.00 | 55.80 | 6 |
| 5 | ATOM | 1763 | CB | ARG | B | 15 | 28.271 | 39.239 | 7.183 | 1.00 | 56.87 | 6 |
| | ATOM | 1764 | CG | ARG | B | 15 | 28.540 | 39.145 | 5.684 | 1.00 | 60.72 | 6 |
| | ATOM | 1765 | CD | ARG | B | 15 | 27.721 | 40.179 | 4.945 | 1.00 | 63.19 | 6 |
| | ATOM | 1766 | NE | ARG | B | 15 | 28.008 | 41.515 | 5.475 | 1.00 | 67.21 | 7 |
| | ATOM | 1767 | CZ | ARG | B | 15 | 27.307 | 42.616 | 5.196 | 1.00 | 67.82 | 6 |
| 10 | ATOM | 1768 | NH1 | ARG | B | 15 | 26.259 | 42.549 | 4.384 | 1.00 | 69.12 | 7 |
| | ATOM | 1769 | NH2 | ARG | B | 15 | 27.660 | 43.789 | 5.722 | 1.00 | 66.84 | 7 |
| | ATOM | 1770 | C | ARG | B | 15 | 28.962 | 38.655 | 9.511 | 1.00 | 54.09 | 6 |
| | ATOM | 1771 | O | ARG | B | 15 | 27.795 | 38.651 | 9.880 | 1.00 | 55.59 | 8 |
| | ATOM | 1772 | N | PRO | B | 16 | 29.979 | 38.747 | 10.377 | 1.00 | 51.42 | 7 |
| 15 | ATOM | 1773 | CD | PRO | B | 16 | 31.405 | 38.751 | 10.015 | 1.00 | 48.17 | 6 |
| | ATOM | 1774 | CA | PRO | B | 16 | 29.817 | 38.846 | 11.828 | 1.00 | 48.94 | 6 |
| | ATOM | 1775 | CB | PRO | B | 16 | 31.256 | 38.950 | 12.328 | 1.00 | 48.44 | 6 |
| | ATOM | 1776 | CG | PRO | B | 16 | 32.038 | 38.262 | 11.284 | 1.00 | 48.62 | 6 |
| | ATOM | 1777 | C | PRO | B | 16 | 28.974 | 40.014 | 12.300 | 1.00 | 48.35 | 6 |
| 20 | ATOM | 1778 | O | PRO | B | 16 | 28.475 | 40.006 | 13.420 | 1.00 | 49.87 | 8 |
| | ATOM | 1779 | N | ASP | B | 17 | 28.825 | 41.026 | 11.456 | 1.00 | 49.55 | 7 |
| | ATOM | 1780 | CA | ASP | B | 17 | 28.048 | 42.201 | 11.830 | 1.00 | 51.87 | 6 |
| | ATOM | 1781 | CB | ASP | B | 17 | 28.638 | 43.469 | 11.204 | 1.00 | 55.73 | 6 |
| | ATOM | 1782 | CG | ASP | B | 17 | 29.956 | 43.896 | 11.856 | 1.00 | 59.93 | 6 |
| 25 | ATOM | 1783 | OD1 | ASP | B | 17 | 30.158 | 43.598 | 13.062 | 1.00 | 60.57 | 8 |
| | ATOM | 1784 | OD2 | ASP | B | 17 | 30.781 | 44.548 | 11.163 | 1.00 | 61.01 | 8 |
| | ATOM | 1785 | C | ASP | B | 17 | 26.581 | 42.120 | 11.458 | 1.00 | 51.65 | 6 |
| | ATOM | 1786 | O | ASP | B | 17 | 25.837 | 43.066 | 11.684 | 1.00 | 51.12 | 8 |
| | ATOM | 1787 | N | VAL | B | 18 | 26.156 | 40.990 | 10.906 | 1.00 | 53.24 | 7 |
| 30 | ATOM | 1788 | CA | VAL | B | 18 | 24.772 | 40.848 | 10.495 | 1.00 | 53.38 | 6 |
| | ATOM | 1789 | CB | VAL | B | 18 | 24.679 | 40.682 | 8.978 | 1.00 | 52.53 | 6 |
| | ATOM | 1790 | CG1 | VAL | B | 18 | 23.238 | 40.628 | 8.551 | 1.00 | 53.33 | 6 |
| | ATOM | 1791 | CG2 | VAL | B | 18 | 25.385 | 41.833 | 8.299 | 1.00 | 52.08 | 6 |
| | ATOM | 1792 | C | VAL | B | 18 | 24.026 | 39.701 | 11.157 | 1.00 | 54.80 | 6 |
| 35 | ATOM | 1793 | O | VAL | B | 18 | 24.359 | 38.527 | 10.980 | 1.00 | 57.05 | 8 |
| | ATOM | 1794 | N | ILE | B | 19 | 22.999 | 40.062 | 11.913 | 1.00 | 55.38 | 7 |
| | ATOM | 1795 | CA | ILE | B | 19 | 22.150 | 39.105 | 12.615 | 1.00 | 54.84 | 6 |
| | ATOM | 1796 | CB | ILE | B | 19 | 21.128 | 39.899 | 13.493 | 1.00 | 53.97 | 6 |
| | ATOM | 1797 | CG2 | ILE | B | 19 | 20.177 | 40.699 | 12.612 | 1.00 | 52.99 | 6 |
| 40 | ATOM | 1798 | CG1 | ILE | B | 19 | 20.354 | 38.963 | 14.414 | 1.00 | 54.58 | 6 |
| | ATOM | 1799 | CD1 | ILE | B | 19 | 19.598 | 39.696 | 15.490 | 1.00 | 51.38 | 6 |
| | ATOM | 1800 | C | ILE | B | 19 | 21.450 | 38.192 | 11.586 | 1.00 | 55.77 | 6 |
| | ATOM | 1801 | O | ILE | B | 19 | 20.879 | 38.678 | 10.605 | 1.00 | 56.23 | 8 |
| | ATOM | 1802 | N | PRO | B | 20 | 21.508 | 36.857 | 11.787 | 1.00 | 57.54 | 7 |
| 45 | ATOM | 1803 | CD | PRO | B | 20 | 22.223 | 36.204 | 12.888 | 1.00 | 57.31 | 6 |
| | ATOM | 1804 | CA | PRO | B | 20 | 20.900 | 35.841 | 10.900 | 1.00 | 59.26 | 6 |
| | ATOM | 1805 | CB | PRO | B | 20 | 21.478 | 34.521 | 11.417 | 1.00 | 57.46 | 6 |
| | ATOM | 1806 | CG | PRO | B | 20 | 22.657 | 34.935 | 12.235 | 1.00 | 58.77 | 6 |
| | ATOM | 1807 | C | PRO | B | 20 | 19.366 | 35.836 | 10.940 | 1.00 | 62.02 | 6 |
| 50 | ATOM | 1808 | O | PRO | B | 20 | 18.732 | 34.806 | 11.185 | 1.00 | 61.74 | 8 |
| | ATOM | 1809 | N | THR | B | 21 | 18.781 | 36.997 | 10.679 | 1.00 | 65.81 | 7 |
| | ATOM | 1810 | CA | THR | B | 21 | 17.337 | 37.160 | 10.705 | 1.00 | 69.72 | 6 |
| | ATOM | 1811 | CB | THR | B | 21 | 16.974 | 38.658 | 10.971 | 1.00 | 67.96 | 6 |
| | ATOM | 1812 | OG1 | THR | B | 21 | 16.710 | 38.837 | 12.367 | 1.00 | 69.51 | 8 |
| 55 | ATOM | 1813 | CG2 | THR | B | 21 | 15.765 | 39.087 | 10.178 | 1.00 | 68.09 | 6 |
| | ATOM | 1814 | C | THR | B | 21 | 16.606 | 36.658 | 9.455 | 1.00 | 73.11 | 6 |
| | ATOM | 1815 | O | THR | B | 21 | 17.000 | 36.942 | 8.315 | 1.00 | 71.83 | 8 |
| | ATOM | 1816 | N | GLN | B | 22 | 15.532 | 35.907 | 9.694 | 1.00 | 77.49 | 7 |
| | ATOM | 1817 | CA | GLN | B | 22 | 14.684 | 35.370 | 8.629 | 1.00 | 80.52 | 6 |
| 60 | ATOM | 1818 | CB | GLN | B | 22 | 14.492 | 33.871 | 8.842 | 1.00 | 81.72 | 6 |
| | ATOM | 1819 | CG | GLN | B | 22 | 15.793 | 33.097 | 8.917 | 1.00 | 83.16 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 1820 | CD | GLN | B | 22 | 15.654 | 31.832 | 9.753 | 1.00 | 85.69 | 6 |
| | ATOM | 1821 | OE1 | GLN | B | 22 | 15.421 | 31.901 | 10.976 | 1.00 | 86.08 | 8 |
| | ATOM | 1822 | NE2 | GLN | B | 22 | 15.787 | 30.665 | 9.103 | 1.00 | 85.85 | 7 |
| | ATOM | 1823 | C | GLN | B | 22 | 13.326 | 36.091 | 8.717 | 1.00 | 81.72 | 6 |
| 5 | ATOM | 1824 | O | GLN | B | 22 | 12.526 | 35.837 | 9.632 | 1.00 | 80.46 | 8 |
| | ATOM | 1825 | N | ARG | B | 23 | 13.075 | 36.990 | 7.765 | 1.00 | 84.00 | 7 |
| | ATOM | 1826 | CA | ARG | B | 23 | 11.829 | 37.769 | 7.744 | 1.00 | 86.23 | 6 |
| | ATOM | 1827 | CB | ARG | B | 23 | 10.599 | 36.840 | 7.695 | 1.00 | 87.50 | 6 |
| | ATOM | 1828 | CG | ARG | B | 23 | 10.348 | 36.215 | 6.314 | 1.00 | 89.89 | 6 |
| 10 | ATOM | 1829 | CD | ARG | B | 23 | 10.796 | 34.734 | 6.215 | 1.00 | 90.83 | 6 |
| | ATOM | 1830 | NE | ARG | B | 23 | 10.694 | 34.242 | 4.833 | 1.00 | 93.76 | 7 |
| | ATOM | 1831 | CZ | ARG | B | 23 | 9.590 | 34.302 | 4.068 | 1.00 | 95.64 | 6 |
| | ATOM | 1832 | NH1 | ARG | B | 23 | 8.452 | 34.832 | 4.534 | 1.00 | 96.17 | 7 |
| | ATOM | 1833 | NH2 | ARG | B | 23 | 9.627 | 33.855 | 2.811 | 1.00 | 95.03 | 7 |
| 15 | ATOM | 1834 | C | ARG | B | 23 | 11.754 | 38.657 | 8.987 | 1.00 | 86.03 | 6 |
| | ATOM | 1835 | O | ARG | B | 23 | 12.776 | 39.137 | 9.476 | 1.00 | 85.87 | 8 |
| | ATOM | 1836 | N | ASP | B | 24 | 10.548 | 38.879 | 9.497 | 1.00 | 86.08 | 7 |
| | ATOM | 1837 | CA | ASP | B | 24 | 10.393 | 39.703 | 10.693 | 1.00 | 85.72 | 6 |
| | ATOM | 1838 | CB | ASP | B | 24 | 8.975 | 40.301 | 10.799 | 1.00 | 89.17 | 6 |
| 20 | ATOM | 1839 | CG | ASP | B | 24 | 8.226 | 40.339 | 9.453 | 1.00 | 90.77 | 6 |
| | ATOM | 1840 | OD1 | ASP | B | 24 | 8.743 | 40.965 | 8.486 | 1.00 | 92.05 | 8 |
| | ATOM | 1841 | OD2 | ASP | B | 24 | 7.113 | 39.746 | 9.376 | 1.00 | 89.95 | 8 |
| | ATOM | 1842 | C | ASP | B | 24 | 10.622 | 38.798 | 11.891 | 1.00 | 83.93 | 6 |
| | ATOM | 1843 | O | ASP | B | 24 | 10.445 | 39.218 | 13.045 | 1.00 | 83.66 | 8 |
| 25 | ATOM | 1844 | N | ARG | B | 25 | 10.994 | 37.549 | 11.613 | 1.00 | 81.18 | 7 |
| | ATOM | 1845 | CA | ARG | B | 25 | 11.237 | 36.584 | 12.677 | 1.00 | 78.99 | 6 |
| | ATOM | 1846 | CB | ARG | B | 25 | 11.318 | 35.159 | 12.128 | 1.00 | 82.30 | 6 |
| | ATOM | 1847 | CG | ARG | B | 25 | 10.001 | 34.541 | 11.696 | 1.00 | 87.15 | 6 |
| | ATOM | 1848 | CD | ARG | B | 25 | 10.171 | 33.024 | 11.485 | 1.00 | 91.09 | 6 |
| 30 | ATOM | 1849 | NE | ARG | B | 25 | 8.908 | 32.371 | 11.140 | 1.00 | 95.87 | 7 |
| | ATOM | 1850 | CZ | ARG | B | 25 | 8.747 | 31.053 | 11.005 | 1.00 | 98.43 | 6 |
| | ATOM | 1851 | NH1 | ARG | B | 25 | 9.785 | 30.235 | 11.186 | 1.00 | 97.96 | 7 |
| | ATOM | 1852 | NH2 | ARG | B | 25 | 7.538 | 30.549 | 10.709 | 1.00 | 99.56 | 7 |
| | ATOM | 1853 | C | ARG | B | 25 | 12.527 | 36.876 | 13.426 | 1.00 | 75.18 | 6 |
| 35 | ATOM | 1854 | O | ARG | B | 25 | 13.573 | 37.105 | 12.813 | 1.00 | 75.11 | 8 |
| | ATOM | 1855 | N | PRO | B | 26 | 12.463 | 36.879 | 14.767 | 1.00 | 71.32 | 7 |
| | ATOM | 1856 | CD | PRO | B | 26 | 11.233 | 36.885 | 15.569 | 1.00 | 69.54 | 6 |
| | ATOM | 1857 | CA | PRO | B | 26 | 13.629 | 37.134 | 15.617 | 1.00 | 68.20 | 6 |
| | ATOM | 1858 | CB | PRO | B | 26 | 13.020 | 37.298 | 17.007 | 1.00 | 68.04 | 6 |
| 40 | ATOM | 1859 | CG | PRO | B | 26 | 11.627 | 37.763 | 16.720 | 1.00 | 68.94 | 6 |
| | ATOM | 1860 | C | PRO | B | 26 | 14.543 | 35.917 | 15.572 | 1.00 | 65.66 | 6 |
| | ATOM | 1861 | O | PRO | B | 26 | 14.114 | 34.832 | 15.183 | 1.00 | 65.23 | 8 |
| | ATOM | 1862 | N | VAL | B | 27 | 15.801 | 36.093 | 15.956 | 1.00 | 62.13 | 7 |
| | ATOM | 1863 | CA | VAL | B | 27 | 16.716 | 34.969 | 15.990 | 1.00 | 58.35 | 6 |
| 45 | ATOM | 1864 | CB | VAL | B | 27 | 18.185 | 35.416 | 15.851 | 1.00 | 57.74 | 6 |
| | ATOM | 1865 | CG1 | VAL | B | 27 | 19.127 | 34.308 | 16.328 | 1.00 | 54.93 | 6 |
| | ATOM | 1866 | CG2 | VAL | B | 27 | 18.479 | 35.737 | 14.393 | 1.00 | 54.94 | 6 |
| | ATOM | 1867 | C | VAL | B | 27 | 16.491 | 34.348 | 17.349 | 1.00 | 56.29 | 6 |
| | ATOM | 1868 | O | VAL | B | 27 | 16.517 | 35.043 | 18.360 | 1.00 | 56.31 | 8 |
| 50 | ATOM | 1869 | N | ALA | B | 28 | 16.243 | 33.045 | 17.379 | 1.00 | 54.44 | 7 |
| | ATOM | 1870 | CA | ALA | B | 28 | 16.008 | 32.384 | 18.645 | 1.00 | 52.98 | 6 |
| | ATOM | 1871 | CB | ALA | B | 28 | 15.095 | 31.209 | 18.461 | 1.00 | 52.15 | 6 |
| | ATOM | 1872 | C | ALA | B | 28 | 17.318 | 31.938 | 19.262 | 1.00 | 52.73 | 6 |
| | ATOM | 1873 | O | ALA | B | 28 | 17.959 | 31.004 | 18.782 | 1.00 | 51.86 | 8 |
| 55 | ATOM | 1874 | N | VAL | B | 29 | 17.696 | 32.632 | 20.334 | 1.00 | 51.10 | 7 |
| | ATOM | 1875 | CA | VAL | B | 29 | 18.911 | 32.353 | 21.080 | 1.00 | 49.08 | 6 |
| | ATOM | 1876 | CB | VAL | B | 29 | 19.741 | 33.642 | 21.324 | 1.00 | 49.72 | 6 |
| | ATOM | 1877 | CG1 | VAL | B | 29 | 20.986 | 33.323 | 22.140 | 1.00 | 46.43 | 6 |
| | ATOM | 1878 | CG2 | VAL | B | 29 | 20.117 | 34.272 | 19.996 | 1.00 | 49.12 | 6 |
| 60 | ATOM | 1879 | C | VAL | B | 29 | 18.553 | 31.762 | 22.428 | 1.00 | 48.65 | 6 |
| | ATOM | 1880 | O | VAL | B | 29 | 17.731 | 32.301 | 23.161 | 1.00 | 48.71 | 8 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 1881 | N | SER | B | 30 | 19.169 | 30.638 | 22.746 | 1.00 | 50.09 | 7 |
| | ATOM | 1882 | CA | SER | B | 30 | 18.925 | 29.997 | 24.018 | 1.00 | 53.68 | 6 |
| | ATOM | 1883 | CB | SER | B | 30 | 18.587 | 28.521 | 23.817 | 1.00 | 53.36 | 6 |
| | ATOM | 1884 | OG | SER | B | 30 | 19.653 | 27.845 | 23.180 | 1.00 | 57.88 | 8 |
| 5 | ATOM | 1885 | C | SER | B | 30 | 20.201 | 30.150 | 24.823 | 1.00 | 56.00 | 6 |
| | ATOM | 1886 | O | SER | B | 30 | 21.297 | 29.933 | 24.306 | 1.00 | 57.56 | 8 |
| | ATOM | 1887 | N | VAL | B | 31 | 20.049 | 30.542 | 26.084 | 1.00 | 57.69 | 7 |
| | ATOM | 1888 | CA | VAL | B | 31 | 21.175 | 30.752 | 26.980 | 1.00 | 57.19 | 6 |
| | ATOM | 1889 | CB | VAL | B | 31 | 21.227 | 32.198 | 27.460 | 1.00 | 57.32 | 6 |
| 10 | ATOM | 1890 | CG1 | VAL | B | 31 | 22.536 | 32.449 | 28.185 | 1.00 | 58.47 | 6 |
| | ATOM | 1891 | CG2 | VAL | B | 31 | 21.044 | 33.147 | 26.288 | 1.00 | 56.64 | 6 |
| | ATOM | 1892 | C | VAL | B | 31 | 21.016 | 29.878 | 28.204 | 1.00 | 57.98 | 6 |
| | ATOM | 1893 | O | VAL | B | 31 | 19.938 | 29.815 | 28.787 | 1.00 | 59.53 | 8 |
| | ATOM | 1894 | N | SER | B | 32 | 22.101 | 29.232 | 28.611 | 1.00 | 58.26 | 7 |
| 15 | ATOM | 1895 | CA | SER | B | 32 | 22.069 | 28.356 | 29.765 | 1.00 | 58.30 | 6 |
| | ATOM | 1896 | CB | SER | B | 32 | 21.806 | 26.914 | 29.298 | 1.00 | 60.26 | 6 |
| | ATOM | 1897 | OG | SER | B | 32 | 21.881 | 25.975 | 30.361 | 1.00 | 61.39 | 8 |
| | ATOM | 1898 | C | SER | B | 32 | 23.374 | 28.414 | 30.530 | 1.00 | 58.22 | 6 |
| | ATOM | 1899 | O | SER | B | 32 | 24.402 | 27.983 | 30.024 | 1.00 | 62.28 | 8 |
| 20 | ATOM | 1900 | N | LEU | B | 33 | 23.340 | 28.937 | 31.753 | 1.00 | 56.90 | 7 |
| | ATOM | 1901 | CA | LEU | B | 33 | 24.548 | 29.002 | 32.572 | 1.00 | 56.09 | 6 |
| | ATOM | 1902 | CB | LEU | B | 33 | 24.489 | 30.183 | 33.541 | 1.00 | 54.84 | 6 |
| | ATOM | 1903 | CG | LEU | B | 33 | 24.257 | 31.555 | 32.914 | 1.00 | 55.33 | 6 |
| | ATOM | 1904 | CD1 | LEU | B | 33 | 24.483 | 32.647 | 33.962 | 1.00 | 53.97 | 6 |
| 25 | ATOM | 1905 | CD2 | LEU | B | 33 | 25.201 | 31.731 | 31.737 | 1.00 | 56.27 | 6 |
| | ATOM | 1906 | C | LEU | B | 33 | 24.725 | 27.728 | 33.379 | 1.00 | 55.50 | 6 |
| | ATOM | 1907 | O | LEU | B | 33 | 23.770 | 27.220 | 33.950 | 1.00 | 56.54 | 8 |
| | ATOM | 1908 | N | LYS | B | 34 | 25.948 | 27.215 | 33.413 | 1.00 | 55.65 | 7 |
| | ATOM | 1909 | CA | LYS | B | 34 | 26.270 | 26.018 | 34.183 | 1.00 | 56.27 | 6 |
| 30 | ATOM | 1910 | CB | LYS | B | 34 | 26.815 | 24.905 | 33.279 | 1.00 | 60.64 | 6 |
| | ATOM | 1911 | CG | LYS | B | 34 | 25.908 | 24.528 | 32.102 | 1.00 | 66.07 | 6 |
| | ATOM | 1912 | CD | LYS | B | 34 | 24.552 | 23.965 | 32.566 | 1.00 | 72.18 | 6 |
| | ATOM | 1913 | CE | LYS | B | 34 | 23.611 | 23.670 | 31.373 | 1.00 | 74.46 | 6 |
| | ATOM | 1914 | NZ | LYS | B | 34 | 22.303 | 23.068 | 31.799 | 1.00 | 74.04 | 7 |
| 35 | ATOM | 1915 | C | LYS | B | 34 | 27.365 | 26.493 | 35.108 | 1.00 | 54.54 | 6 |
| | ATOM | 1916 | O | LYS | B | 34 | 28.463 | 26.811 | 34.655 | 1.00 | 55.93 | 8 |
| | ATOM | 1917 | N | PHE | B | 35 | 27.079 | 26.564 | 36.401 | 1.00 | 52.21 | 7 |
| | ATOM | 1918 | CA | PHE | B | 35 | 28.086 | 27.045 | 37.336 | 1.00 | 49.54 | 6 |
| | ATOM | 1919 | CB | PHE | B | 35 | 27.422 | 27.491 | 38.633 | 1.00 | 46.23 | 6 |
| 40 | ATOM | 1920 | CG | PHE | B | 35 | 26.545 | 28.682 | 38.450 | 1.00 | 47.55 | 6 |
| | ATOM | 1921 | CD1 | PHE | B | 35 | 25.230 | 28.536 | 38.035 | 1.00 | 48.89 | 6 |
| | ATOM | 1922 | CD2 | PHE | B | 35 | 27.056 | 29.968 | 38.603 | 1.00 | 48.56 | 6 |
| | ATOM | 1923 | CE1 | PHE | B | 35 | 24.434 | 29.653 | 37.771 | 1.00 | 47.34 | 6 |
| | ATOM | 1924 | CE2 | PHE | B | 35 | 26.269 | 31.087 | 38.343 | 1.00 | 45.87 | 6 |
| 45 | ATOM | 1925 | CZ | PHE | B | 35 | 24.958 | 30.927 | 37.926 | 1.00 | 47.81 | 6 |
| | ATOM | 1926 | C | PHE | B | 35 | 29.224 | 26.072 | 37.595 | 1.00 | 49.37 | 6 |
| | ATOM | 1927 | O | PHE | B | 35 | 29.020 | 24.880 | 37.833 | 1.00 | 48.82 | 8 |
| | ATOM | 1928 | N | ILE | B | 36 | 30.434 | 26.609 | 37.530 | 1.00 | 47.17 | 7 |
| | ATOM | 1929 | CA | ILE | B | 36 | 31.634 | 25.820 | 37.706 | 1.00 | 45.02 | 6 |
| 50 | ATOM | 1930 | CB | ILE | B | 36 | 32.641 | 26.106 | 36.574 | 1.00 | 42.09 | 6 |
| | ATOM | 1931 | CG2 | ILE | B | 36 | 33.858 | 25.230 | 36.717 | 1.00 | 38.48 | 6 |
| | ATOM | 1932 | CG1 | ILE | B | 36 | 31.966 | 25.897 | 35.224 | 1.00 | 41.05 | 6 |
| | ATOM | 1933 | CD1 | ILE | B | 36 | 31.393 | 24.520 | 35.028 | 1.00 | 41.45 | 6 |
| | ATOM | 1934 | C | ILE | B | 36 | 32.284 | 26.141 | 39.029 | 1.00 | 45.51 | 6 |
| 55 | ATOM | 1935 | O | ILE | B | 36 | 32.977 | 25.304 | 39.603 | 1.00 | 45.83 | 8 |
| | ATOM | 1936 | N | ASN | B | 37 | 32.068 | 27.351 | 39.522 | 1.00 | 45.06 | 7 |
| | ATOM | 1937 | CA | ASN | B | 37 | 32.678 | 27.719 | 40.792 | 1.00 | 45.81 | 6 |
| | ATOM | 1938 | CB | ASN | B | 37 | 34.200 | 27.712 | 40.652 | 1.00 | 43.65 | 6 |
| | ATOM | 1939 | CG | ASN | B | 37 | 34.900 | 27.384 | 41.950 | 1.00 | 47.86 | 6 |
| 60 | ATOM | 1940 | OD1 | ASN | B | 37 | 34.518 | 27.864 | 43.025 | 1.00 | 49.43 | 8 |
| | ATOM | 1941 | ND2 | ASN | B | 37 | 35.942 | 26.572 | 41.862 | 1.00 | 46.99 | 7 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 1942 | C | ASN | B | 37 | 32.222 | 29.077 | 41.322 | 1.00 | 45.58 | 6 |
| | ATOM | 1943 | O | ASN | B | 37 | 31.767 | 29.931 | 40.566 | 1.00 | 44.62 | 8 |
| | ATOM | 1944 | N | ILE | B | 38 | 32.335 | 29.248 | 42.635 | 1.00 | 45.83 | 7 |
| | ATOM | 1945 | CA | ILE | B | 38 | 31.973 | 30.489 | 43.301 | 1.00 | 47.98 | 6 |
| 5 | ATOM | 1946 | CB | ILE | B | 38 | 30.781 | 30.287 | 44.214 | 1.00 | 46.41 | 6 |
| | ATOM | 1947 | CG2 | ILE | B | 38 | 30.510 | 31.550 | 44.976 | 1.00 | 46.45 | 6 |
| | ATOM | 1948 | CG1 | ILE | B | 38 | 29.567 | 29.905 | 43.356 | 1.00 | 47.23 | 6 |
| | ATOM | 1949 | CD1 | ILE | B | 38 | 28.365 | 29.406 | 44.105 | 1.00 | 48.96 | 6 |
| 10 | ATOM | 1950 | C | ILE | B | 38 | 33.221 | 30.805 | 44.086 | 1.00 | 50.65 | 6 |
| | ATOM | 1951 | O | ILE | B | 38 | 33.546 | 30.109 | 45.040 | 1.00 | 52.37 | 8 |
| | ATOM | 1952 | N | LEU | B | 39 | 33.926 | 31.855 | 43.668 | 1.00 | 52.96 | 7 |
| | ATOM | 1953 | CA | LEU | B | 39 | 35.207 | 32.214 | 44.264 | 1.00 | 53.68 | 6 |
| | ATOM | 1954 | CB | LEU | B | 39 | 36.137 | 32.698 | 43.157 | 1.00 | 53.70 | 6 |
| | ATOM | 1955 | CG | LEU | B | 39 | 36.204 | 31.706 | 42.000 | 1.00 | 53.99 | 6 |
| 15 | ATOM | 1956 | CD1 | LEU | B | 39 | 37.099 | 32.257 | 40.904 | 1.00 | 53.07 | 6 |
| | ATOM | 1957 | CD2 | LEU | B | 39 | 36.718 | 30.364 | 42.510 | 1.00 | 51.88 | 6 |
| | ATOM | 1958 | C | LEU | B | 39 | 35.272 | 33.188 | 45.418 | 1.00 | 54.85 | 6 |
| | ATOM | 1959 | O | LEU | B | 39 | 36.061 | 32.994 | 46.342 | 1.00 | 55.07 | 8 |
| 20 | ATOM | 1960 | N | GLU | B | 40 | 34.489 | 34.255 | 45.359 | 1.00 | 55.18 | 7 |
| | ATOM | 1961 | CA | GLU | B | 40 | 34.509 | 35.220 | 46.446 | 1.00 | 58.32 | 6 |
| | ATOM | 1962 | CB | GLU | B | 40 | 35.423 | 36.400 | 46.144 | 1.00 | 59.68 | 6 |
| | ATOM | 1963 | CG | GLU | B | 40 | 36.879 | 36.041 | 46.018 | 1.00 | 65.11 | 6 |
| | ATOM | 1964 | CD | GLU | B | 40 | 37.749 | 37.271 | 45.846 | 1.00 | 69.72 | 6 |
| 25 | ATOM | 1965 | OE1 | GLU | B | 40 | 37.534 | 38.034 | 44.867 | 1.00 | 72.04 | 8 |
| | ATOM | 1966 | OE2 | GLU | B | 40 | 38.648 | 37.477 | 46.693 | 1.00 | 70.63 | 8 |
| | ATOM | 1967 | C | GLU | B | 40 | 33.128 | 35.738 | 46.685 | 1.00 | 59.54 | 6 |
| | ATOM | 1968 | O | GLU | B | 40 | 32.393 | 36.057 | 45.747 | 1.00 | 59.65 | 8 |
| | ATOM | 1969 | N | VAL | B | 41 | 32.772 | 35.816 | 47.956 | 1.00 | 60.26 | 7 |
| 30 | ATOM | 1970 | CA | VAL | B | 41 | 31.468 | 36.304 | 48.323 | 1.00 | 58.68 | 6 |
| | ATOM | 1971 | CB | VAL | B | 41 | 30.599 | 35.159 | 48.862 | 1.00 | 59.00 | 6 |
| | ATOM | 1972 | CG1 | VAL | B | 41 | 29.318 | 35.711 | 49.450 | 1.00 | 61.18 | 6 |
| | ATOM | 1973 | CG2 | VAL | B | 41 | 30.279 | 34.186 | 47.740 | 1.00 | 59.58 | 6 |
| | ATOM | 1974 | C | VAL | B | 41 | 31.666 | 37.368 | 49.379 | 1.00 | 58.15 | 6 |
| 35 | ATOM | 1975 | O | VAL | B | 41 | 32.594 | 37.290 | 50.187 | 1.00 | 56.97 | 8 |
| | ATOM | 1976 | N | ASN | B | 42 | 30.811 | 38.383 | 49.337 | 1.00 | 58.17 | 7 |
| | ATOM | 1977 | CA | ASN | B | 42 | 30.863 | 39.466 | 50.302 | 1.00 | 58.74 | 6 |
| | ATOM | 1978 | CB | ASN | B | 42 | 31.609 | 40.673 | 49.730 | 1.00 | 58.84 | 6 |
| | ATOM | 1979 | CG | ASN | B | 42 | 31.962 | 41.702 | 50.795 | 1.00 | 58.68 | 6 |
| 40 | ATOM | 1980 | OD1 | ASN | B | 42 | 31.122 | 42.100 | 51.593 | 1.00 | 58.91 | 8 |
| | ATOM | 1981 | ND2 | ASN | B | 42 | 33.215 | 42.138 | 50.806 | 1.00 | 58.72 | 7 |
| | ATOM | 1982 | C | ASN | B | 42 | 29.412 | 39.823 | 50.577 | 1.00 | 60.60 | 6 |
| | ATOM | 1983 | O | ASN | B | 42 | 28.738 | 40.457 | 49.747 | 1.00 | 60.01 | 8 |
| | ATOM | 1984 | N | GLU | B | 43 | 28.926 | 39.401 | 51.742 | 1.00 | 61.86 | 7 |
| 45 | ATOM | 1985 | CA | GLU | B | 43 | 27.543 | 39.669 | 52.111 | 1.00 | 62.81 | 6 |
| | ATOM | 1986 | CB | GLU | B | 43 | 27.117 | 38.760 | 53.267 | 1.00 | 64.87 | 6 |
| | ATOM | 1987 | CG | GLU | B | 43 | 25.640 | 38.871 | 53.591 | 1.00 | 67.01 | 6 |
| | ATOM | 1988 | CD | GLU | B | 43 | 25.152 | 37.779 | 54.525 | 1.00 | 69.52 | 6 |
| | ATOM | 1989 | OE1 | GLU | B | 43 | 23.973 | 37.842 | 54.945 | 1.00 | 68.10 | 8 |
| 50 | ATOM | 1990 | OE2 | GLU | B | 43 | 25.944 | 36.854 | 54.831 | 1.00 | 70.46 | 8 |
| | ATOM | 1991 | C | GLU | B | 43 | 27.332 | 41.132 | 52.476 | 1.00 | 60.60 | 6 |
| | ATOM | 1992 | O | GLU | B | 43 | 26.223 | 41.649 | 52.387 | 1.00 | 59.23 | 8 |
| | ATOM | 1993 | N | ILE | B | 44 | 28.408 | 41.792 | 52.882 | 1.00 | 60.18 | 7 |
| | ATOM | 1994 | CA | ILE | B | 44 | 28.356 | 43.199 | 53.254 | 1.00 | 61.54 | 6 |
| | ATOM | 1995 | CB | ILE | B | 44 | 29.674 | 43.669 | 53.910 | 1.00 | 62.98 | 6 |
| 55 | ATOM | 1996 | CG2 | ILE | B | 44 | 29.601 | 45.172 | 54.183 | 1.00 | 61.14 | 6 |
| | ATOM | 1997 | CG1 | ILE | B | 44 | 29.950 | 42.877 | 55.194 | 1.00 | 63.64 | 6 |
| | ATOM | 1998 | CD1 | ILE | B | 44 | 29.004 | 43.205 | 56.335 | 1.00 | 65.05 | 6 |
| | ATOM | 1999 | C | ILE | B | 44 | 28.141 | 44.069 | 52.016 | 1.00 | 62.14 | 6 |
| 60 | ATOM | 2000 | O | ILE | B | 44 | 27.318 | 44.992 | 52.024 | 1.00 | 62.54 | 8 |
| | ATOM | 2001 | N | THR | B | 45 | 28.894 | 43.773 | 50.959 | 1.00 | 60.63 | 7 |
| | ATOM | 2002 | CA | THR | B | 45 | 28.806 | 44.527 | 49.721 | 1.00 | 59.11 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2003 | CB | THR | B | 45 | 30.190 | 44.696 | 49.090 | 1.00 | 58.49 | 6 |
| | ATOM | 2004 | OG1 | THR | B | 45 | 30.749 | 43.403 | 48.815 | 1.00 | 60.11 | 8 |
| | ATOM | 2005 | CG2 | THR | B | 45 | 31.106 | 45.444 | 50.036 | 1.00 | 56.17 | 6 |
| | ATOM | 2006 | C | THR | B | 45 | 27.879 | 43.894 | 48.688 | 1.00 | 58.30 | 6 |
| | ATOM | 2007 | O | THR | B | 45 | 27.555 | 44.521 | 47.675 | 1.00 | 58.45 | 8 |
| 10 | ATOM | 2008 | N | ASN | B | 46 | 27.450 | 42.660 | 48.933 | 1.00 | 56.14 | 7 |
| | ATOM | 2009 | CA | ASN | B | 46 | 26.560 | 42.001 | 47.986 | 1.00 | 55.54 | 6 |
| | ATOM | 2010 | CB | ASN | B | 46 | 25.242 | 42.770 | 47.894 | 1.00 | 54.26 | 6 |
| | ATOM | 2011 | CG | ASN | B | 46 | 24.161 | 42.171 | 48.767 | 1.00 | 56.06 | 6 |
| | ATOM | 2012 | OD1 | ASN | B | 46 | 23.195 | 42.835 | 49.103 | 1.00 | 55.63 | 8 |
| 15 | ATOM | 2013 | ND2 | ASN | B | 46 | 24.314 | 40.898 | 49.123 | 1.00 | 56.99 | 7 |
| | ATOM | 2014 | C | ASN | B | 46 | 27.190 | 41.867 | 46.591 | 1.00 | 54.59 | 6 |
| | ATOM | 2015 | O | ASN | B | 46 | 26.589 | 42.228 | 45.574 | 1.00 | 52.67 | 8 |
| | ATOM | 2016 | N | GLU | B | 47 | 28.408 | 41.337 | 46.565 | 1.00 | 53.06 | 7 |
| | ATOM | 2017 | CA | GLU | B | 47 | 29.141 | 41.131 | 45.330 | 1.00 | 51.52 | 6 |
| 20 | ATOM | 2018 | CB | GLU | B | 47 | 30.320 | 42.090 | 45.267 | 1.00 | 49.41 | 6 |
| | ATOM | 2019 | CG | GLU | B | 47 | 29.902 | 43.534 | 45.211 | 1.00 | 51.44 | 6 |
| | ATOM | 2020 | CD | GLU | B | 47 | 31.084 | 44.472 | 45.232 | 1.00 | 53.91 | 6 |
| | ATOM | 2021 | OE1 | GLU | B | 47 | 32.183 | 44.015 | 44.862 | 1.00 | 51.27 | 8 |
| | ATOM | 2022 | OE2 | GLU | B | 47 | 30.911 | 45.662 | 45.604 | 1.00 | 58.92 | 8 |
| 25 | ATOM | 2023 | C | GLU | B | 47 | 29.627 | 39.697 | 45.262 | 1.00 | 50.23 | 6 |
| | ATOM | 2024 | O | GLU | B | 47 | 30.100 | 39.150 | 46.245 | 1.00 | 50.97 | 8 |
| | ATOM | 2025 | N | VAL | B | 48 | 29.509 | 39.090 | 44.091 | 1.00 | 50.68 | 7 |
| | ATOM | 2026 | CA | VAL | B | 48 | 29.928 | 37.706 | 43.909 | 1.00 | 50.46 | 6 |
| | ATOM | 2027 | CB | VAL | B | 48 | 28.712 | 36.793 | 43.633 | 1.00 | 49.57 | 6 |
| 30 | ATOM | 2028 | CG1 | VAL | B | 48 | 29.162 | 35.370 | 43.440 | 1.00 | 53.01 | 6 |
| | ATOM | 2029 | CG2 | VAL | B | 48 | 27.749 | 36.861 | 44.781 | 1.00 | 50.46 | 6 |
| | ATOM | 2030 | C | VAL | B | 48 | 30.910 | 37.554 | 42.757 | 1.00 | 49.70 | 6 |
| | ATOM | 2031 | O | VAL | B | 48 | 30.785 | 38.204 | 41.727 | 1.00 | 50.33 | 8 |
| | ATOM | 2032 | N | ASP | B | 49 | 31.891 | 36.688 | 42.950 | 1.00 | 48.84 | 7 |
| 35 | ATOM | 2033 | CA | ASP | B | 49 | 32.888 | 36.414 | 41.935 | 1.00 | 49.56 | 6 |
| | ATOM | 2034 | CB | ASP | B | 49 | 34.283 | 36.610 | 42.514 | 1.00 | 51.66 | 6 |
| | ATOM | 2035 | CG | ASP | B | 49 | 35.320 | 36.772 | 41.456 | 1.00 | 50.41 | 6 |
| | ATOM | 2036 | OD1 | ASP | B | 49 | 35.214 | 36.073 | 40.443 | 1.00 | 52.66 | 8 |
| | ATOM | 2037 | OD2 | ASP | B | 49 | 36.240 | 37.586 | 41.639 | 1.00 | 51.65 | 8 |
| 40 | ATOM | 2038 | C | ASP | B | 49 | 32.648 | 34.949 | 41.590 | 1.00 | 49.62 | 6 |
| | ATOM | 2039 | O | ASP | B | 49 | 32.973 | 34.052 | 42.364 | 1.00 | 49.38 | 8 |
| | ATOM | 2040 | N | VAL | B | 50 | 32.078 | 34.720 | 40.416 | 1.00 | 49.68 | 7 |
| | ATOM | 2041 | CA | VAL | B | 50 | 31.721 | 33.381 | 39.982 | 1.00 | 48.91 | 6 |
| | ATOM | 2042 | CB | VAL | B | 50 | 30.168 | 33.242 | 40.000 | 1.00 | 50.39 | 6 |
| 45 | ATOM | 2043 | CG1 | VAL | B | 50 | 29.565 | 33.968 | 38.807 | 1.00 | 47.68 | 6 |
| | ATOM | 2044 | CG2 | VAL | B | 50 | 29.767 | 31.781 | 40.006 | 1.00 | 52.12 | 6 |
| | ATOM | 2045 | C | VAL | B | 50 | 32.241 | 32.978 | 38.598 | 1.00 | 47.99 | 6 |
| | ATOM | 2046 | O | VAL | B | 50 | 32.533 | 33.824 | 37.758 | 1.00 | 48.54 | 8 |
| | ATOM | 2047 | N | VAL | B | 51 | 32.349 | 31.669 | 38.383 | 1.00 | 45.73 | 7 |
| 50 | ATOM | 2048 | CA | VAL | B | 51 | 32.802 | 31.091 | 37.116 | 1.00 | 44.16 | 6 |
| | ATOM | 2049 | CB | VAL | B | 51 | 34.037 | 30.178 | 37.313 | 1.00 | 43.78 | 6 |
| | ATOM | 2050 | CG1 | VAL | B | 51 | 34.324 | 29.416 | 36.031 | 1.00 | 40.41 | 6 |
| | ATOM | 2051 | CG2 | VAL | B | 51 | 35.245 | 31.005 | 37.728 | 1.00 | 40.89 | 6 |
| | ATOM | 2052 | C | VAL | B | 51 | 31.673 | 30.227 | 36.569 | 1.00 | 45.01 | 6 |
| 55 | ATOM | 2053 | O | VAL | B | 51 | 31.075 | 29.458 | 37.318 | 1.00 | 48.28 | 8 |
| | ATOM | 2054 | N | PHE | B | 52 | 31.382 | 30.328 | 35.275 | 1.00 | 42.51 | 7 |
| | ATOM | 2055 | CA | PHE | B | 52 | 30.307 | 29.535 | 34.708 | 1.00 | 41.24 | 6 |
| | ATOM | 2056 | CB | PHE | B | 52 | 28.981 | 30.224 | 34.993 | 1.00 | 41.72 | 6 |
| | ATOM | 2057 | CG | PHE | B | 52 | 28.876 | 31.595 | 34.394 | 1.00 | 42.31 | 6 |
| 60 | ATOM | 2058 | CD1 | PHE | B | 52 | 28.448 | 31.767 | 33.088 | 1.00 | 42.63 | 6 |
| | ATOM | 2059 | CD2 | PHE | B | 52 | 29.248 | 32.711 | 35.123 | 1.00 | 43.12 | 6 |
| | ATOM | 2060 | CE1 | PHE | B | 52 | 28.394 | 33.025 | 32.521 | 1.00 | 43.87 | 6 |
| | ATOM | 2061 | CE2 | PHE | B | 52 | 29.197 | 33.976 | 34.562 | 1.00 | 43.32 | 6 |
| | ATOM | 2062 | CZ | PHE | B | 52 | 28.770 | 34.132 | 33.261 | 1.00 | 43.87 | 6 |
| | ATOM | 2063 | C | PHE | B | 52 | 30.463 | 29.345 | 33.217 | 1.00 | 43.44 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 2064 | O | PHE | B | 52 | 31.264 | 30.008 | 32.585 | 1.00 | 46.26 | 8 |
| | ATOM | 2065 | N | TRP | B | 53 | 29.692 | 28.428 | 32.655 | 1.00 | 44.90 | 7 |
| | ATOM | 2066 | CA | TRP | B | 53 | 29.725 | 28.188 | 31.223 | 1.00 | 47.46 | 6 |
| 5 | ATOM | 2067 | CB | TRP | B | 53 | 29.655 | 26.698 | 30.907 | 1.00 | 47.31 | 6 |
| | ATOM | 2068 | CG | TRP | B | 53 | 30.869 | 25.949 | 31.278 | 1.00 | 49.36 | 6 |
| | ATOM | 2069 | CD2 | TRP | B | 53 | 31.029 | 24.535 | 31.246 | 1.00 | 50.82 | 6 |
| | ATOM | 2070 | CE2 | TRP | B | 53 | 32.342 | 24.253 | 31.686 | 1.00 | 49.80 | 6 |
| | ATOM | 2071 | CE3 | TRP | B | 53 | 30.189 | 23.473 | 30.887 | 1.00 | 51.30 | 6 |
| | ATOM | 2072 | CD1 | TRP | B | 53 | 32.057 | 26.463 | 31.719 | 1.00 | 50.05 | 6 |
| 10 | ATOM | 2073 | NE1 | TRP | B | 53 | 32.947 | 25.448 | 31.968 | 1.00 | 50.43 | 7 |
| | ATOM | 2074 | CZ2 | TRP | B | 53 | 32.835 | 22.955 | 31.779 | 1.00 | 50.23 | 6 |
| | ATOM | 2075 | CZ3 | TRP | B | 53 | 30.676 | 22.182 | 30.977 | 1.00 | 49.78 | 6 |
| | ATOM | 2076 | CH2 | TRP | B | 53 | 31.990 | 21.932 | 31.421 | 1.00 | 50.88 | 6 |
| | ATOM | 2077 | C | TRP | B | 53 | 28.516 | 28.860 | 30.619 | 1.00 | 48.93 | 6 |
| 15 | ATOM | 2078 | O | TRP | B | 53 | 27.388 | 28.490 | 30.912 | 1.00 | 48.69 | 8 |
| | ATOM | 2079 | N | GLN | B | 54 | 28.746 | 29.846 | 29.770 | 1.00 | 50.46 | 7 |
| | ATOM | 2080 | CA | GLN | B | 54 | 27.643 | 30.543 | 29.155 | 1.00 | 51.66 | 6 |
| | ATOM | 2081 | CB | GLN | B | 54 | 28.036 | 31.984 | 28.844 | 1.00 | 51.35 | 6 |
| | ATOM | 2082 | CG | GLN | B | 54 | 26.871 | 32.851 | 28.407 | 1.00 | 53.49 | 6 |
| 20 | ATOM | 2083 | CD | GLN | B | 54 | 27.117 | 34.326 | 28.693 | 1.00 | 57.50 | 6 |
| | ATOM | 2084 | OE1 | GLN | B | 54 | 27.399 | 34.711 | 29.837 | 1.00 | 57.95 | 8 |
| | ATOM | 2085 | NE2 | GLN | B | 54 | 27.016 | 35.161 | 27.659 | 1.00 | 58.04 | 7 |
| | ATOM | 2086 | C | GLN | B | 54 | 27.273 | 29.790 | 27.898 | 1.00 | 52.38 | 6 |
| | ATOM | 2087 | O | GLN | B | 54 | 27.564 | 30.209 | 26.786 | 1.00 | 54.42 | 8 |
| 25 | ATOM | 2088 | N | GLN | B | 55 | 26.638 | 28.650 | 28.101 | 1.00 | 52.78 | 7 |
| | ATOM | 2089 | CA | GLN | B | 55 | 26.203 | 27.793 | 27.017 | 1.00 | 53.84 | 6 |
| | ATOM | 2090 | CB | GLN | B | 55 | 25.672 | 26.501 | 27.623 | 1.00 | 58.14 | 6 |
| | ATOM | 2091 | CG | GLN | B | 55 | 24.985 | 25.549 | 26.663 | 1.00 | 66.74 | 6 |
| | ATOM | 2092 | CD | GLN | B | 55 | 24.756 | 24.190 | 27.315 | 1.00 | 70.87 | 6 |
| 30 | ATOM | 2093 | OE1 | GLN | B | 55 | 24.456 | 24.108 | 28.528 | 1.00 | 73.46 | 8 |
| | ATOM | 2094 | NE2 | GLN | B | 55 | 24.897 | 23.117 | 26.527 | 1.00 | 69.32 | 7 |
| | ATOM | 2095 | C | GLN | B | 55 | 25.145 | 28.495 | 26.168 | 1.00 | 51.37 | 6 |
| | ATOM | 2096 | O | GLN | B | 55 | 23.993 | 28.631 | 26.563 | 1.00 | 52.24 | 8 |
| | ATOM | 2097 | N | THR | B | 56 | 25.558 | 28.935 | 24.989 | 1.00 | 48.92 | 7 |
| 35 | ATOM | 2098 | CA | THR | B | 56 | 24.690 | 29.660 | 24.083 | 1.00 | 47.03 | 6 |
| | ATOM | 2099 | CB | THR | B | 56 | 25.307 | 31.018 | 23.741 | 1.00 | 47.18 | 6 |
| | ATOM | 2100 | OG1 | THR | B | 56 | 25.758 | 31.647 | 24.946 | 1.00 | 46.91 | 8 |
| | ATOM | 2101 | CG2 | THR | B | 56 | 24.291 | 31.909 | 23.056 | 1.00 | 45.50 | 6 |
| | ATOM | 2102 | C | THR | B | 56 | 24.466 | 28.896 | 22.787 | 1.00 | 46.66 | 6 |
| 40 | ATOM | 2103 | O | THR | B | 56 | 25.351 | 28.202 | 22.306 | 1.00 | 46.60 | 8 |
| | ATOM | 2104 | N | THR | B | 57 | 23.273 | 29.034 | 22.220 | 1.00 | 45.86 | 7 |
| | ATOM | 2105 | CA | THR | B | 57 | 22.942 | 28.350 | 20.984 | 1.00 | 44.53 | 6 |
| | ATOM | 2106 | CB | THR | B | 57 | 22.320 | 26.958 | 21.247 | 1.00 | 44.84 | 6 |
| | ATOM | 2107 | OG1 | THR | B | 57 | 23.271 | 26.115 | 21.910 | 1.00 | 41.11 | 8 |
| 45 | ATOM | 2108 | CG2 | THR | B | 57 | 21.942 | 26.306 | 19.936 | 1.00 | 46.63 | 6 |
| | ATOM | 2109 | C | THR | B | 57 | 21.967 | 29.152 | 20.162 | 1.00 | 43.27 | 6 |
| | ATOM | 2110 | O | THR | B | 57 | 21.106 | 29.825 | 20.700 | 1.00 | 44.01 | 8 |
| | ATOM | 2111 | N | TRP | B | 58 | 22.122 | 29.086 | 18.849 | 1.00 | 41.40 | 7 |
| | ATOM | 2112 | CA | TRP | B | 58 | 21.235 | 29.792 | 17.945 | 1.00 | 42.18 | 6 |
| 50 | ATOM | 2113 | CB | TRP | B | 58 | 21.500 | 31.302 | 17.968 | 1.00 | 40.63 | 6 |
| | ATOM | 2114 | CG | TRP | B | 58 | 22.800 | 31.729 | 17.377 | 1.00 | 40.64 | 6 |
| | ATOM | 2115 | CD2 | TRP | B | 58 | 24.048 | 31.827 | 18.054 | 1.00 | 37.47 | 6 |
| | ATOM | 2116 | CE2 | TRP | B | 58 | 24.998 | 32.252 | 17.113 | 1.00 | 37.44 | 6 |
| | ATOM | 2117 | CE3 | TRP | B | 58 | 24.456 | 31.594 | 19.371 | 1.00 | 37.69 | 6 |
| 55 | ATOM | 2118 | CD1 | TRP | B | 58 | 23.036 | 32.088 | 16.087 | 1.00 | 39.23 | 6 |
| | ATOM | 2119 | NE1 | TRP | B | 58 | 24.354 | 32.404 | 15.917 | 1.00 | 36.19 | 7 |
| | ATOM | 2120 | CZ2 | TRP | B | 58 | 26.336 | 32.452 | 17.444 | 1.00 | 40.36 | 6 |
| | ATOM | 2121 | CZ3 | TRP | B | 58 | 25.778 | 31.789 | 19.701 | 1.00 | 38.85 | 6 |
| | ATOM | 2122 | CH2 | TRP | B | 58 | 26.708 | 32.215 | 18.742 | 1.00 | 40.16 | 6 |
| 60 | ATOM | 2123 | C | TRP | B | 58 | 21.430 | 29.217 | 16.561 | 1.00 | 43.00 | 6 |
| | ATOM | 2124 | O | TRP | B | 58 | 22.226 | 28.320 | 16.383 | 1.00 | 44.24 | 8 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2125 | N | SER | B | 59 | 20.711 | 29.729 | 15.579 | 1.00 | 47.57 | 7 |
| | ATOM | 2126 | CA | SER | B | 59 | 20.814 | 29.181 | 14.246 | 1.00 | 50.36 | 6 |
| | ATOM | 2127 | CB | SER | B | 59 | 19.517 | 28.410 | 13.937 | 1.00 | 52.43 | 6 |
| | ATOM | 2128 | OG | SER | B | 59 | 19.677 | 27.455 | 12.901 | 1.00 | 58.14 | 8 |
| | ATOM | 2129 | C | SER | B | 59 | 21.073 | 30.250 | 13.191 | 1.00 | 51.80 | 6 |
| 10 | ATOM | 2130 | O | SER | B | 59 | 20.440 | 31.307 | 13.184 | 1.00 | 48.66 | 8 |
| | ATOM | 2131 | N | ASP | B | 60 | 22.018 | 29.954 | 12.303 | 1.00 | 53.93 | 7 |
| | ATOM | 2132 | CA | ASP | B | 60 | 22.393 | 30.844 | 11.206 | 1.00 | 56.01 | 6 |
| | ATOM | 2133 | CB | ASP | B | 60 | 23.766 | 31.462 | 11.474 | 1.00 | 57.13 | 6 |
| | ATOM | 2134 | CG | ASP | B | 60 | 24.163 | 32.503 | 10.437 | 1.00 | 58.21 | 6 |
| 15 | ATOM | 2135 | OD1 | ASP | B | 60 | 23.714 | 32.413 | 9.275 | 1.00 | 56.08 | 8 |
| | ATOM | 2136 | OD2 | ASP | B | 60 | 24.952 | 33.407 | 10.786 | 1.00 | 59.82 | 8 |
| | ATOM | 2137 | C | ASP | B | 60 | 22.453 | 29.976 | 9.953 | 1.00 | 57.25 | 6 |
| | ATOM | 2138 | O | ASP | B | 60 | 23.458 | 29.315 | 9.683 | 1.00 | 57.02 | 8 |
| | ATOM | 2139 | N | ARG | B | 61 | 21.370 | 29.979 | 9.192 | 1.00 | 59.51 | 7 |
| 20 | ATOM | 2140 | CA | ARG | B | 61 | 21.281 | 29.171 | 7.981 | 1.00 | 62.14 | 6 |
| | ATOM | 2141 | CB | ARG | B | 61 | 19.852 | 29.202 | 7.418 | 1.00 | 65.88 | 6 |
| | ATOM | 2142 | CG | ARG | B | 61 | 18.842 | 28.288 | 8.125 | 1.00 | 71.80 | 6 |
| | ATOM | 2143 | CD | ARG | B | 61 | 17.562 | 28.189 | 7.282 | 1.00 | 79.30 | 6 |
| | ATOM | 2144 | NE | ARG | B | 61 | 16.561 | 27.245 | 7.806 | 1.00 | 85.93 | 7 |
| 25 | ATOM | 2145 | CZ | ARG | B | 61 | 15.393 | 26.967 | 7.210 | 1.00 | 88.02 | 6 |
| | ATOM | 2146 | NH1 | ARG | B | 61 | 15.059 | 27.553 | 6.059 | 1.00 | 89.55 | 7 |
| | ATOM | 2147 | NH2 | ARG | B | 61 | 14.550 | 26.101 | 7.762 | 1.00 | 88.72 | 7 |
| | ATOM | 2148 | C | ARG | B | 61 | 22.256 | 29.537 | 6.868 | 1.00 | 61.20 | 6 |
| | ATOM | 2149 | O | ARG | B | 61 | 22.488 | 28.725 | 5.972 | 1.00 | 61.95 | 8 |
| 30 | ATOM | 2150 | N | THR | B | 62 | 22.819 | 30.742 | 6.898 | 1.00 | 59.72 | 7 |
| | ATOM | 2151 | CA | THR | B | 62 | 23.755 | 31.133 | 5.846 | 1.00 | 59.39 | 6 |
| | ATOM | 2152 | CB | THR | B | 62 | 24.072 | 32.653 | 5.878 | 1.00 | 61.53 | 6 |
| | ATOM | 2153 | OG1 | THR | B | 62 | 24.790 | 32.981 | 7.077 | 1.00 | 62.67 | 8 |
| | ATOM | 2154 | CG2 | THR | B | 62 | 22.783 | 33.461 | 5.826 | 1.00 | 61.46 | 6 |
| 35 | ATOM | 2155 | C | THR | B | 62 | 25.055 | 30.355 | 5.992 | 1.00 | 58.40 | 6 |
| | ATOM | 2156 | O | THR | B | 62 | 25.923 | 30.410 | 5.129 | 1.00 | 58.95 | 8 |
| | ATOM | 2157 | N | LEU | B | 63 | 25.176 | 29.626 | 7.095 | 1.00 | 57.74 | 7 |
| | ATOM | 2158 | CA | LEU | B | 63 | 26.365 | 28.831 | 7.381 | 1.00 | 55.00 | 6 |
| | ATOM | 2159 | CB | LEU | B | 63 | 26.677 | 28.871 | 8.880 | 1.00 | 53.55 | 6 |
| 40 | ATOM | 2160 | CG | LEU | B | 63 | 26.908 | 30.230 | 9.531 | 1.00 | 52.72 | 6 |
| | ATOM | 2161 | CD1 | LEU | B | 63 | 27.061 | 30.070 | 11.038 | 1.00 | 53.77 | 6 |
| | ATOM | 2162 | CD2 | LEU | B | 63 | 28.141 | 30.866 | 8.929 | 1.00 | 52.77 | 6 |
| | ATOM | 2163 | C | LEU | B | 63 | 26.163 | 27.377 | 6.971 | 1.00 | 54.84 | 6 |
| | ATOM | 2164 | O | LEU | B | 63 | 27.125 | 26.624 | 6.858 | 1.00 | 55.28 | 8 |
| 45 | ATOM | 2165 | N | ALA | B | 64 | 24.911 | 26.986 | 6.767 | 1.00 | 53.09 | 7 |
| | ATOM | 2166 | CA | ALA | B | 64 | 24.579 | 25.621 | 6.403 | 1.00 | 54.25 | 6 |
| | ATOM | 2167 | CB | ALA | B | 64 | 23.078 | 25.474 | 6.274 | 1.00 | 54.84 | 6 |
| | ATOM | 2168 | C | ALA | B | 64 | 25.235 | 25.173 | 5.116 | 1.00 | 54.35 | 6 |
| | ATOM | 2169 | O | ALA | B | 64 | 25.441 | 25.973 | 4.208 | 1.00 | 56.81 | 8 |
| 50 | ATOM | 2170 | N | TRP | B | 65 | 25.543 | 23.884 | 5.040 | 1.00 | 50.85 | 7 |
| | ATOM | 2171 | CA | TRP | B | 65 | 26.148 | 23.305 | 3.851 | 1.00 | 50.36 | 6 |
| | ATOM | 2172 | CB | TRP | B | 65 | 27.674 | 23.449 | 3.895 | 1.00 | 47.85 | 6 |
| | ATOM | 2173 | CG | TRP | B | 65 | 28.356 | 22.496 | 4.836 | 1.00 | 44.59 | 6 |
| | ATOM | 2174 | CD2 | TRP | B | 65 | 28.626 | 22.704 | 6.229 | 1.00 | 42.42 | 6 |
| 55 | ATOM | 2175 | CE2 | TRP | B | 65 | 29.244 | 21.535 | 6.711 | 1.00 | 41.31 | 6 |
| | ATOM | 2176 | CE3 | TRP | B | 65 | 28.406 | 23.766 | 7.115 | 1.00 | 39.86 | 6 |
| | ATOM | 2177 | CD1 | TRP | B | 65 | 28.809 | 21.247 | 4.544 | 1.00 | 43.65 | 6 |
| | ATOM | 2178 | NE1 | TRP | B | 65 | 29.344 | 20.664 | 5.662 | 1.00 | 42.95 | 7 |
| | ATOM | 2179 | CZ2 | TRP | B | 65 | 29.645 | 21.393 | 8.041 | 1.00 | 41.27 | 6 |
| 60 | ATOM | 2180 | CZ3 | TRP | B | 65 | 28.807 | 23.624 | 8.439 | 1.00 | 39.24 | 6 |
| | ATOM | 2181 | CH2 | TRP | B | 65 | 29.419 | 22.445 | 8.886 | 1.00 | 40.26 | 6 |
| | ATOM | 2182 | C | TRP | B | 65 | 25.751 | 21.835 | 3.839 | 1.00 | 51.92 | 6 |
| | ATOM | 2183 | O | TRP | B | 65 | 25.269 | 21.312 | 4.846 | 1.00 | 51.65 | 8 |
| | ATOM | 2184 | N | ASN | B | 66 | 25.933 | 21.173 | 2.703 | 1.00 | 54.28 | 7 |
| | ATOM | 2185 | CA | ASN | B | 66 | 25.579 | 19.760 | 2.599 | 1.00 | 56.88 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 2186 | CB | ASN | B | 66 | 25.361 | 19.349 | 1.139 | 1.00 | 59.16 | 6 |
| | ATOM | 2187 | CG | ASN | B | 66 | 25.067 | 17.869 | 1.006 | 1.00 | 62.92 | 6 |
| | ATOM | 2188 | OD1 | ASN | B | 66 | 25.084 | 17.308 | -0.090 | 1.00 | 64.20 | 8 |
| | ATOM | 2189 | ND2 | ASN | B | 66 | 24.792 | 17.223 | 2.138 | 1.00 | 63.82 | 7 |
| 5 | ATOM | 2190 | C | ASN | B | 66 | 26.684 | 18.903 | 3.197 | 1.00 | 56.22 | 6 |
| | ATOM | 2191 | O | ASN | B | 66 | 27.826 | 18.942 | 2.747 | 1.00 | 54.74 | 8 |
| | ATOM | 2192 | N | SER | B | 67 | 26.336 | 18.112 | 4.200 | 1.00 | 57.45 | 7 |
| | ATOM | 2193 | CA | SER | B | 67 | 27.323 | 17.276 | 4.866 | 1.00 | 60.21 | 6 |
| | ATOM | 2194 | CB | SER | B | 67 | 27.251 | 17.503 | 6.376 | 1.00 | 60.70 | 6 |
| 10 | ATOM | 2195 | OG | SER | B | 67 | 25.956 | 17.197 | 6.844 | 1.00 | 59.26 | 8 |
| | ATOM | 2196 | C | SER | B | 67 | 27.139 | 15.796 | 4.554 | 1.00 | 60.90 | 6 |
| | ATOM | 2197 | O | SER | B | 67 | 27.705 | 14.926 | 5.221 | 1.00 | 59.74 | 8 |
| | ATOM | 2198 | N | SER | B | 68 | 26.350 | 15.519 | 3.528 | 1.00 | 62.89 | 7 |
| | ATOM | 2199 | CA | SER | B | 68 | 26.094 | 14.148 | 3.129 | 1.00 | 64.44 | 6 |
| 15 | ATOM | 2200 | CB | SER | B | 68 | 25.141 | 14.127 | 1.933 | 1.00 | 64.07 | 6 |
| | ATOM | 2201 | OG | SER | B | 68 | 25.569 | 15.023 | 0.923 | 1.00 | 65.05 | 8 |
| | ATOM | 2202 | C | SER | B | 68 | 27.399 | 13.437 | 2.790 | 1.00 | 65.22 | 6 |
| | ATOM | 2203 | O | SER | B | 68 | 27.491 | 12.215 | 2.898 | 1.00 | 65.18 | 8 |
| | ATOM | 2204 | N | HIS | B | 69 | 28.414 | 14.203 | 2.401 | 1.00 | 66.21 | 7 |
| 20 | ATOM | 2205 | CA | HIS | B | 69 | 29.702 | 13.617 | 2.054 | 1.00 | 66.70 | 6 |
| | ATOM | 2206 | CB | HIS | B | 69 | 29.832 | 13.502 | 0.539 | 1.00 | 69.64 | 6 |
| | ATOM | 2207 | CG | HIS | B | 69 | 29.047 | 12.363 | -0.025 | 1.00 | 74.89 | 6 |
| | ATOM | 2208 | CD2 | HIS | B | 69 | 29.433 | 11.123 | -0.417 | 1.00 | 76.05 | 6 |
| | ATOM | 2209 | ND1 | HIS | B | 69 | 27.673 | 12.393 | -0.143 | 1.00 | 76.35 | 7 |
| 25 | ATOM | 2210 | CE1 | HIS | B | 69 | 27.245 | 11.221 | -0.583 | 1.00 | 76.49 | 6 |
| | ATOM | 2211 | NE2 | HIS | B | 69 | 28.293 | 10.433 | -0.757 | 1.00 | 76.65 | 7 |
| | ATOM | 2212 | C | HIS | B | 69 | 30.895 | 14.352 | 2.633 | 1.00 | 65.56 | 6 |
| | ATOM | 2213 | O | HIS | B | 69 | 31.919 | 14.538 | 1.971 | 1.00 | 63.93 | 8 |
| | ATOM | 2214 | N | SER | B | 70 | 30.746 | 14.737 | 3.897 | 1.00 | 65.07 | 7 |
| 30 | ATOM | 2215 | CA | SER | B | 70 | 31.772 | 15.463 | 4.632 | 1.00 | 63.00 | 6 |
| | ATOM | 2216 | CB | SER | B | 70 | 31.954 | 16.854 | 4.004 | 1.00 | 61.97 | 6 |
| | ATOM | 2217 | OG | SER | B | 70 | 30.716 | 17.393 | 3.551 | 1.00 | 59.22 | 8 |
| | ATOM | 2218 | C | SER | B | 70 | 31.353 | 15.576 | 6.105 | 1.00 | 62.92 | 6 |
| | ATOM | 2219 | O | SER | B | 70 | 30.288 | 15.077 | 6.507 | 1.00 | 62.73 | 8 |
| 35 | ATOM | 2220 | N | PRO | B | 71 | 32.204 | 16.199 | 6.937 | 1.00 | 62.42 | 7 |
| | ATOM | 2221 | CD | PRO | B | 71 | 33.624 | 16.490 | 6.672 | 1.00 | 61.13 | 6 |
| | ATOM | 2222 | CA | PRO | B | 71 | 31.901 | 16.371 | 8.361 | 1.00 | 61.29 | 6 |
| | ATOM | 2223 | CB | PRO | B | 71 | 33.124 | 17.103 | 8.879 | 1.00 | 61.30 | 6 |
| | ATOM | 2224 | CG | PRO | B | 71 | 34.214 | 16.490 | 8.063 | 1.00 | 60.40 | 6 |
| 40 | ATOM | 2225 | C | PRO | B | 71 | 30.619 | 17.159 | 8.575 | 1.00 | 61.12 | 6 |
| | ATOM | 2226 | O | PRO | B | 71 | 30.222 | 17.964 | 7.733 | 1.00 | 60.52 | 8 |
| | ATOM | 2227 | N | ASP | B | 72 | 29.973 | 16.916 | 9.708 | 1.00 | 62.69 | 7 |
| | ATOM | 2228 | CA | ASP | B | 72 | 28.714 | 17.587 | 10.046 | 1.00 | 62.55 | 6 |
| | ATOM | 2229 | CB | ASP | B | 72 | 27.839 | 16.649 | 10.883 | 1.00 | 64.34 | 6 |
| 45 | ATOM | 2230 | CG | ASP | B | 72 | 27.143 | 15.613 | 10.040 | 1.00 | 67.53 | 6 |
| | ATOM | 2231 | OD1 | ASP | B | 72 | 25.937 | 15.794 | 9.767 | 1.00 | 67.60 | 8 |
| | ATOM | 2232 | OD2 | ASP | B | 72 | 27.808 | 14.627 | 9.631 | 1.00 | 70.97 | 8 |
| | ATOM | 2233 | C | ASP | B | 72 | 28.962 | 18.858 | 10.827 | 1.00 | 60.43 | 6 |
| | ATOM | 2234 | O | ASP | B | 72 | 28.137 | 19.780 | 10.815 | 1.00 | 58.20 | 8 |
| 50 | ATOM | 2235 | N | GLN | B | 73 | 30.123 | 18.883 | 11.483 | 1.00 | 58.87 | 7 |
| | ATOM | 2236 | CA | GLN | B | 73 | 30.549 | 19.981 | 12.339 | 1.00 | 58.03 | 6 |
| | ATOM | 2237 | CB | GLN | B | 73 | 30.400 | 19.583 | 13.788 | 1.00 | 60.56 | 6 |
| | ATOM | 2238 | CG | GLN | B | 73 | 29.025 | 19.532 | 14.346 | 1.00 | 62.56 | 6 |
| | ATOM | 2239 | CD | GLN | B | 73 | 29.096 | 19.033 | 15.763 | 1.00 | 64.10 | 6 |
| 55 | ATOM | 2240 | OE1 | GLN | B | 73 | 29.599 | 17.945 | 16.003 | 1.00 | 67.42 | 8 |
| | ATOM | 2241 | NE2 | GLN | B | 73 | 28.628 | 19.830 | 16.711 | 1.00 | 65.84 | 7 |
| | ATOM | 2242 | C | GLN | B | 73 | 31.998 | 20.392 | 12.165 | 1.00 | 55.43 | 6 |
| | ATOM | 2243 | O | GLN | B | 73 | 32.845 | 19.591 | 11.754 | 1.00 | 56.41 | 8 |
| | ATOM | 2244 | N | VAL | B | 74 | 32.275 | 21.642 | 12.522 | 1.00 | 50.91 | 7 |
| 60 | ATOM | 2245 | CA | VAL | B | 74 | 33.621 | 22.197 | 12.464 | 1.00 | 48.23 | 6 |
| | ATOM | 2246 | CB | VAL | B | 74 | 33.925 | 22.849 | 11.107 | 1.00 | 46.99 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 2247 | CG1 | VAL | B | 74 | 34.009 | 21.782 | 10.026 | 1.00 | 48.63 | 6 |
| | ATOM | 2248 | CG2 | VAL | B | 74 | 32.864 | 23.871 | 10.777 | 1.00 | 45.41 | 6 |
| | ATOM | 2249 | C | VAL | B | 74 | 33.734 | 23.259 | 13.532 | 1.00 | 46.89 | 6 |
| | ATOM | 2250 | O | VAL | B | 74 | 32.731 | 23.812 | 13.964 | 1.00 | 46.87 | 8 |
| 5 | ATOM | 2251 | N | SER | B | 75 | 34.951 | 23.524 | 13.980 | 1.00 | 44.18 | 7 |
| | ATOM | 2252 | CA | SER | B | 75 | 35.177 | 24.551 | 14.982 | 1.00 | 41.30 | 6 |
| | ATOM | 2253 | CB | SER | B | 75 | 36.314 | 24.145 | 15.920 | 1.00 | 39.05 | 6 |
| | ATOM | 2254 | OG | SER | B | 75 | 35.850 | 23.290 | 16.932 | 1.00 | 30.94 | 8 |
| | ATOM | 2255 | C | SER | B | 75 | 35.513 | 25.856 | 14.264 | 1.00 | 40.02 | 6 |
| 10 | ATOM | 2256 | O | SER | B | 75 | 36.478 | 25.936 | 13.516 | 1.00 | 39.74 | 8 |
| | ATOM | 2257 | N | VAL | B | 76 | 34.701 | 26.875 | 14.497 | 1.00 | 39.53 | 7 |
| | ATOM | 2258 | CA | VAL | B | 76 | 34.885 | 28.167 | 13.861 | 1.00 | 40.26 | 6 |
| | ATOM | 2259 | CB | VAL | B | 76 | 33.607 | 28.580 | 13.124 | 1.00 | 42.73 | 6 |
| | ATOM | 2260 | CG1 | VAL | B | 76 | 33.788 | 29.928 | 12.483 | 1.00 | 43.36 | 6 |
| 15 | ATOM | 2261 | CG2 | VAL | B | 76 | 33.244 | 27.539 | 12.090 | 1.00 | 40.50 | 6 |
| | ATOM | 2262 | C | VAL | B | 76 | 35.218 | 29.256 | 14.861 | 1.00 | 40.57 | 6 |
| | ATOM | 2263 | O | VAL | B | 76 | 34.626 | 29.322 | 15.926 | 1.00 | 41.80 | 8 |
| | ATOM | 2264 | N | PRO | B | 77 | 36.188 | 30.120 | 14.541 | 1.00 | 40.43 | 7 |
| | ATOM | 2265 | CD | PRO | B | 77 | 37.176 | 30.053 | 13.460 | 1.00 | 39.25 | 6 |
| 20 | ATOM | 2266 | CA | PRO | B | 77 | 36.527 | 31.189 | 15.479 | 1.00 | 39.73 | 6 |
| | ATOM | 2267 | CB | PRO | B | 77 | 37.717 | 31.853 | 14.816 | 1.00 | 40.77 | 6 |
| | ATOM | 2268 | CG | PRO | B | 77 | 38.342 | 30.728 | 14.078 | 1.00 | 40.80 | 6 |
| | ATOM | 2269 | C | PRO | B | 77 | 35.346 | 32.141 | 15.622 | 1.00 | 38.02 | 6 |
| | ATOM | 2270 | O | PRO | B | 77 | 34.663 | 32.438 | 14.658 | 1.00 | 39.36 | 8 |
| 25 | ATOM | 2271 | N | ILE | B | 78 | 35.105 | 32.600 | 16.835 | 1.00 | 37.63 | 7 |
| | ATOM | 2272 | CA | ILE | B | 78 | 34.018 | 33.515 | 17.129 | 1.00 | 39.61 | 6 |
| | ATOM | 2273 | CB | ILE | B | 78 | 34.107 | 33.946 | 18.602 | 1.00 | 41.86 | 6 |
| | ATOM | 2274 | CG2 | ILE | B | 78 | 33.311 | 35.183 | 18.861 | 1.00 | 40.86 | 6 |
| | ATOM | 2275 | CG1 | ILE | B | 78 | 33.622 | 32.799 | 19.469 | 1.00 | 45.04 | 6 |
| 30 | ATOM | 2276 | CD1 | ILE | B | 78 | 32.313 | 32.232 | 18.983 | 1.00 | 46.64 | 6 |
| | ATOM | 2277 | C | ILE | B | 78 | 34.000 | 34.741 | 16.231 | 1.00 | 41.00 | 6 |
| | ATOM | 2278 | O | ILE | B | 78 | 32.947 | 35.225 | 15.846 | 1.00 | 41.00 | 8 |
| | ATOM | 2279 | N | SER | B | 79 | 35.185 | 35.227 | 15.898 | 1.00 | 43.87 | 7 |
| | ATOM | 2280 | CA | SER | B | 79 | 35.368 | 36.399 | 15.047 | 1.00 | 44.52 | 6 |
| 35 | ATOM | 2281 | CB | SER | B | 79 | 36.842 | 36.792 | 15.061 | 1.00 | 46.91 | 6 |
| | ATOM | 2282 | OG | SER | B | 79 | 37.657 | 35.687 | 14.696 | 1.00 | 49.85 | 8 |
| | ATOM | 2283 | C | SER | B | 79 | 34.914 | 36.244 | 13.593 | 1.00 | 43.47 | 6 |
| | ATOM | 2284 | O | SER | B | 79 | 34.805 | 37.228 | 12.876 | 1.00 | 43.49 | 8 |
| | ATOM | 2285 | N | SER | B | 80 | 34.656 | 35.016 | 13.160 | 1.00 | 43.24 | 7 |
| 40 | ATOM | 2286 | CA | SER | B | 80 | 34.227 | 34.769 | 11.793 | 1.00 | 44.14 | 6 |
| | ATOM | 2287 | CB | SER | B | 80 | 34.955 | 33.552 | 11.221 | 1.00 | 44.85 | 6 |
| | ATOM | 2288 | OG | SER | B | 80 | 36.354 | 33.781 | 11.115 | 1.00 | 52.06 | 8 |
| | ATOM | 2289 | C | SER | B | 80 | 32.731 | 34.545 | 11.690 | 1.00 | 44.49 | 6 |
| | ATOM | 2290 | O | SER | B | 80 | 32.213 | 34.308 | 10.609 | 1.00 | 44.54 | 8 |
| 45 | ATOM | 2291 | N | LEU | B | 81 | 32.039 | 34.625 | 12.820 | 1.00 | 45.89 | 7 |
| | ATOM | 2292 | CA | LEU | B | 81 | 30.589 | 34.418 | 12.858 | 1.00 | 45.78 | 6 |
| | ATOM | 2293 | CB | LEU | B | 81 | 30.250 | 33.187 | 13.700 | 1.00 | 42.48 | 6 |
| | ATOM | 2294 | CG | LEU | B | 81 | 30.945 | 31.867 | 13.420 | 1.00 | 42.60 | 6 |
| | ATOM | 2295 | CD1 | LEU | B | 81 | 30.769 | 30.949 | 14.584 | 1.00 | 41.27 | 6 |
| 50 | ATOM | 2296 | CD2 | LEU | B | 81 | 30.379 | 31.266 | 12.165 | 1.00 | 45.70 | 6 |
| | ATOM | 2297 | C | LEU | B | 81 | 29.909 | 35.611 | 13.513 | 1.00 | 45.11 | 6 |
| | ATOM | 2298 | O | LEU | B | 81 | 30.562 | 36.439 | 14.154 | 1.00 | 46.02 | 8 |
| | ATOM | 2299 | N | TRP | B | 82 | 28.596 | 35.696 | 13.344 | 1.00 | 42.92 | 7 |
| | ATOM | 2300 | CA | TRP | B | 82 | 27.829 | 36.737 | 13.984 | 1.00 | 40.24 | 6 |
| 55 | ATOM | 2301 | CB | TRP | B | 82 | 26.493 | 36.962 | 13.290 | 1.00 | 42.22 | 6 |
| | ATOM | 2302 | CG | TRP | B | 82 | 25.535 | 37.766 | 14.126 | 1.00 | 43.85 | 6 |
| | ATOM | 2303 | CD2 | TRP | B | 82 | 24.580 | 37.257 | 15.072 | 1.00 | 44.14 | 6 |
| | ATOM | 2304 | CE2 | TRP | B | 82 | 23.972 | 38.369 | 15.687 | 1.00 | 42.05 | 6 |
| | ATOM | 2305 | CE3 | TRP | B | 82 | 24.185 | 35.964 | 15.461 | 1.00 | 42.43 | 6 |
| 60 | ATOM | 2306 | CD1 | TRP | B | 82 | 25.459 | 39.118 | 14.204 | 1.00 | 42.92 | 6 |
| | ATOM | 2307 | NE1 | TRP | B | 82 | 24.527 | 39.490 | 15.138 | 1.00 | 41.43 | 7 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 2308 | CZ2 | TRP | B | 82 | 22.991 | 38.238 | 16.671 | 1.00 | 42.94 | 6 |
| | ATOM | 2309 | CZ3 | TRP | B | 82 | 23.211 | 35.832 | 16.442 | 1.00 | 41.79 | 6 |
| | ATOM | 2310 | CH2 | TRP | B | 82 | 22.625 | 36.965 | 17.036 | 1.00 | 42.57 | 6 |
| | ATOM | 2311 | C | TRP | B | 82 | 27.579 | 36.100 | 15.323 | 1.00 | 39.43 | 6 |
| 5 | ATOM | 2312 | O | TRP | B | 82 | 27.379 | 34.904 | 15.410 | 1.00 | 41.05 | 8 |
| | ATOM | 2313 | N | VAL | B | 83 | 27.594 | 36.892 | 16.373 | 1.00 | 41.18 | 7 |
| | ATOM | 2314 | CA | VAL | B | 83 | 27.363 | 36.359 | 17.699 | 1.00 | 40.57 | 6 |
| | ATOM | 2315 | CB | VAL | B | 83 | 28.714 | 36.210 | 18.444 | 1.00 | 41.00 | 6 |
| | ATOM | 2316 | CG1 | VAL | B | 83 | 28.494 | 35.956 | 19.903 | 1.00 | 45.57 | 6 |
| 10 | ATOM | 2317 | CG2 | VAL | B | 83 | 29.491 | 35.066 | 17.856 | 1.00 | 40.97 | 6 |
| | ATOM | 2318 | C | VAL | B | 83 | 26.399 | 37.275 | 18.460 | 1.00 | 40.40 | 6 |
| | ATOM | 2319 | O | VAL | B | 83 | 26.424 | 38.487 | 18.301 | 1.00 | 42.78 | 8 |
| | ATOM | 2320 | N | PRO | B | 84 | 25.510 | 36.693 | 19.271 | 1.00 | 40.62 | 7 |
| | ATOM | 2321 | CD | PRO | B | 84 | 25.296 | 35.250 | 19.465 | 1.00 | 43.06 | 6 |
| 15 | ATOM | 2322 | CA | PRO | B | 84 | 24.540 | 37.460 | 20.052 | 1.00 | 39.62 | 6 |
| | ATOM | 2323 | CB | PRO | B | 84 | 23.839 | 36.384 | 20.880 | 1.00 | 39.00 | 6 |
| | ATOM | 2324 | CG | PRO | B | 84 | 23.899 | 35.212 | 20.013 | 1.00 | 43.18 | 6 |
| | ATOM | 2325 | C | PRO | B | 84 | 25.246 | 38.474 | 20.937 | 1.00 | 37.37 | 6 |
| | ATOM | 2326 | O | PRO | B | 84 | 26.215 | 38.140 | 21.603 | 1.00 | 34.20 | 8 |
| 20 | ATOM | 2327 | N | ASP | B | 85 | 24.753 | 39.706 | 20.950 | 1.00 | 36.29 | 7 |
| | ATOM | 2328 | CA | ASP | B | 85 | 25.341 | 40.736 | 21.777 | 1.00 | 37.57 | 6 |
| | ATOM | 2329 | CB | ASP | B | 85 | 25.112 | 42.107 | 21.152 | 1.00 | 38.52 | 6 |
| | ATOM | 2330 | CG | ASP | B | 85 | 23.661 | 42.418 | 20.952 | 1.00 | 40.81 | 6 |
| | ATOM | 2331 | OD1 | ASP | B | 85 | 22.925 | 41.501 | 20.578 | 1.00 | 41.81 | 8 |
| 25 | ATOM | 2332 | OD2 | ASP | B | 85 | 23.254 | 43.579 | 21.148 | 1.00 | 41.12 | 8 |
| | ATOM | 2333 | C | ASP | B | 85 | 24.776 | 40.687 | 23.193 | 1.00 | 39.08 | 6 |
| | ATOM | 2334 | O | ASP | B | 85 | 24.261 | 41.668 | 23.714 | 1.00 | 36.01 | 8 |
| | ATOM | 2335 | N | LEU | B | 86 | 24.902 | 39.522 | 23.811 | 1.00 | 38.19 | 7 |
| | ATOM | 2336 | CA | LEU | B | 86 | 24.421 | 39.306 | 25.161 | 1.00 | 39.63 | 6 |
| 30 | ATOM | 2337 | CB | LEU | B | 86 | 24.459 | 37.819 | 25.502 | 1.00 | 37.18 | 6 |
| | ATOM | 2338 | CG | LEU | B | 86 | 23.585 | 36.939 | 24.621 | 1.00 | 38.33 | 6 |
| | ATOM | 2339 | CD1 | LEU | B | 86 | 23.700 | 35.493 | 25.065 | 1.00 | 33.72 | 6 |
| | ATOM | 2340 | CD2 | LEU | B | 86 | 22.159 | 37.433 | 24.693 | 1.00 | 35.49 | 6 |
| | ATOM | 2341 | C | LEU | B | 86 | 25.223 | 40.061 | 26.201 | 1.00 | 40.05 | 6 |
| 35 | ATOM | 2342 | O | LEU | B | 86 | 26.432 | 40.251 | 26.065 | 1.00 | 42.26 | 8 |
| | ATOM | 2343 | N | ALA | B | 87 | 24.541 | 40.467 | 27.260 | 1.00 | 40.28 | 7 |
| | ATOM | 2344 | CA | ALA | B | 87 | 25.180 | 41.193 | 28.339 | 1.00 | 40.51 | 6 |
| | ATOM | 2345 | CB | ALA | B | 87 | 25.048 | 42.698 | 28.091 | 1.00 | 40.62 | 6 |
| | ATOM | 2346 | C | ALA | B | 87 | 24.521 | 40.826 | 29.660 | 1.00 | 40.28 | 6 |
| 40 | ATOM | 2347 | O | ALA | B | 87 | 23.306 | 40.702 | 29.729 | 1.00 | 40.56 | 8 |
| | ATOM | 2348 | N | ALA | B | 88 | 25.316 | 40.634 | 30.703 | 1.00 | 39.13 | 7 |
| | ATOM | 2349 | CA | ALA | B | 88 | 24.756 | 40.340 | 32.014 | 1.00 | 38.99 | 6 |
| | ATOM | 2350 | CB | ALA | B | 88 | 25.749 | 39.577 | 32.850 | 1.00 | 37.09 | 6 |
| | ATOM | 2351 | C | ALA | B | 88 | 24.433 | 41.686 | 32.665 | 1.00 | 40.68 | 6 |
| 45 | ATOM | 2352 | O | ALA | B | 88 | 25.319 | 42.392 | 33.134 | 1.00 | 38.34 | 8 |
| | ATOM | 2353 | N | TYR | B | 89 | 23.153 | 42.033 | 32.667 | 1.00 | 42.45 | 7 |
| | ATOM | 2354 | CA | TYR | B | 89 | 22.654 | 43.285 | 33.232 | 1.00 | 44.08 | 6 |
| | ATOM | 2355 | CB | TYR | B | 89 | 21.133 | 43.209 | 33.363 | 1.00 | 46.62 | 6 |
| | ATOM | 2356 | CG | TYR | B | 89 | 20.395 | 43.055 | 32.056 | 1.00 | 51.23 | 6 |
| 50 | ATOM | 2357 | CD1 | TYR | B | 89 | 19.022 | 42.816 | 32.036 | 1.00 | 54.25 | 6 |
| | ATOM | 2358 | CE1 | TYR | B | 89 | 18.322 | 42.711 | 30.826 | 1.00 | 55.90 | 6 |
| | ATOM | 2359 | CD2 | TYR | B | 89 | 21.054 | 43.179 | 30.835 | 1.00 | 52.13 | 6 |
| | ATOM | 2360 | CE2 | TYR | B | 89 | 20.366 | 43.078 | 29.626 | 1.00 | 54.28 | 6 |
| | ATOM | 2361 | CZ | TYR | B | 89 | 19.001 | 42.847 | 29.629 | 1.00 | 55.97 | 6 |
| 55 | ATOM | 2362 | OH | TYR | B | 89 | 18.313 | 42.787 | 28.440 | 1.00 | 59.26 | 8 |
| | ATOM | 2363 | C | TYR | B | 89 | 23.243 | 43.725 | 34.579 | 1.00 | 43.48 | 6 |
| | ATOM | 2364 | O | TYR | B | 89 | 23.409 | 44.917 | 34.820 | 1.00 | 42.18 | 8 |
| | ATOM | 2365 | N | ASN | B | 90 | 23.540 | 42.784 | 35.466 | 1.00 | 42.08 | 7 |
| | ATOM | 2366 | CA | ASN | B | 90 | 24.102 | 43.155 | 36.755 | 1.00 | 40.43 | 6 |
| 60 | ATOM | 2367 | CB | ASN | B | 90 | 23.262 | 42.581 | 37.904 | 1.00 | 39.29 | 6 |
| | ATOM | 2368 | CG | ASN | B | 90 | 23.084 | 41.082 | 37.824 | 1.00 | 40.77 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 2369 | OD1 | ASN | B | 90 | 22.778 | 40.536 | 36.774 | 1.00 | 40.90 | 8 |
| | ATOM | 2370 | ND2 | ASN | B | 90 | 23.257 | 40.412 | 38.948 | 1.00 | 42.41 | 7 |
| | ATOM | 2371 | C | ASN | B | 90 | 25.554 | 42.768 | 36.921 | 1.00 | 41.50 | 6 |
| | ATOM | 2372 | O | ASN | B | 90 | 26.031 | 42.618 | 38.042 | 1.00 | 42.85 | 8 |
| 5 | ATOM | 2373 | N | ALA | B | 91 | 26.250 | 42.605 | 35.798 | 1.00 | 43.60 | 7 |
| | ATOM | 2374 | CA | ALA | B | 91 | 27.669 | 42.266 | 35.811 | 1.00 | 43.31 | 6 |
| | ATOM | 2375 | CB | ALA | B | 91 | 28.156 | 41.933 | 34.415 | 1.00 | 42.36 | 6 |
| | ATOM | 2376 | C | ALA | B | 91 | 28.359 | 43.513 | 36.336 | 1.00 | 44.47 | 6 |
| | ATOM | 2377 | O | ALA | B | 91 | 28.048 | 44.637 | 35.934 | 1.00 | 43.75 | 8 |
| 10 | ATOM | 2378 | N | ILE | B | 92 | 29.295 | 43.299 | 37.244 | 1.00 | 44.99 | 7 |
| | ATOM | 2379 | CA | ILE | B | 92 | 30.009 | 44.379 | 37.895 | 1.00 | 45.69 | 6 |
| | ATOM | 2380 | CB | ILE | B | 92 | 30.052 | 44.061 | 39.418 | 1.00 | 46.91 | 6 |
| | ATOM | 2381 | CG2 | ILE | B | 92 | 31.419 | 43.514 | 39.831 | 1.00 | 49.50 | 6 |
| | ATOM | 2382 | CG1 | ILE | B | 92 | 29.726 | 45.288 | 40.232 | 1.00 | 48.64 | 6 |
| 15 | ATOM | 2383 | CD1 | ILE | B | 92 | 29.920 | 45.030 | 41.718 | 1.00 | 53.73 | 6 |
| | ATOM | 2384 | C | ILE | B | 92 | 31.428 | 44.532 | 37.302 | 1.00 | 45.86 | 6 |
| | ATOM | 2385 | O | ILE | B | 92 | 32.156 | 45.487 | 37.611 | 1.00 | 45.24 | 8 |
| | ATOM | 2386 | N | SER | B | 93 | 31.804 | 43.581 | 36.453 | 1.00 | 41.25 | 7 |
| | ATOM | 2387 | CA | SER | B | 93 | 33.104 | 43.578 | 35.813 | 1.00 | 38.58 | 6 |
| 20 | ATOM | 2388 | CB | SER | B | 93 | 34.056 | 42.662 | 36.568 | 1.00 | 35.19 | 6 |
| | ATOM | 2389 | OG | SER | B | 93 | 33.682 | 41.315 | 36.388 | 1.00 | 35.43 | 8 |
| | ATOM | 2390 | C | SER | B | 93 | 32.852 | 43.015 | 34.431 | 1.00 | 40.88 | 6 |
| | ATOM | 2391 | O | SER | B | 93 | 31.776 | 42.493 | 34.174 | 1.00 | 39.63 | 8 |
| | ATOM | 2392 | N | LYS | B | 94 | 33.815 | 43.131 | 33.524 | 1.00 | 43.16 | 7 |
| 25 | ATOM | 2393 | CA | LYS | B | 94 | 33.598 | 42.557 | 32.212 | 1.00 | 43.98 | 6 |
| | ATOM | 2394 | CB | LYS | B | 94 | 34.355 | 43.325 | 31.127 | 1.00 | 46.29 | 6 |
| | ATOM | 2395 | CG | LYS | B | 94 | 35.769 | 43.727 | 31.434 | 1.00 | 50.31 | 6 |
| | ATOM | 2396 | CD | LYS | B | 94 | 36.225 | 44.764 | 30.401 | 1.00 | 52.39 | 6 |
| | ATOM | 2397 | CE | LYS | B | 94 | 35.853 | 44.341 | 28.978 | 1.00 | 52.02 | 6 |
| 30 | ATOM | 2398 | NZ | LYS | B | 94 | 36.333 | 45.308 | 27.965 | 1.00 | 54.82 | 7 |
| | ATOM | 2399 | C | LYS | B | 94 | 33.963 | 41.075 | 32.230 | 1.00 | 43.71 | 6 |
| | ATOM | 2400 | O | LYS | B | 94 | 34.673 | 40.602 | 33.114 | 1.00 | 44.78 | 8 |
| | ATOM | 2401 | N | PRO | B | 95 | 33.443 | 40.310 | 31.267 | 1.00 | 44.16 | 7 |
| | ATOM | 2402 | CD | PRO | B | 95 | 32.562 | 40.750 | 30.171 | 1.00 | 42.37 | 6 |
| 35 | ATOM | 2403 | CA | PRO | B | 95 | 33.704 | 38.873 | 31.184 | 1.00 | 39.82 | 6 |
| | ATOM | 2404 | CB | PRO | B | 95 | 32.836 | 38.422 | 30.016 | 1.00 | 40.83 | 6 |
| | ATOM | 2405 | CG | PRO | B | 95 | 31.813 | 39.505 | 29.881 | 1.00 | 42.58 | 6 |
| | ATOM | 2406 | C | PRO | B | 95 | 35.141 | 38.524 | 30.941 | 1.00 | 39.41 | 6 |
| | ATOM | 2407 | O | PRO | B | 95 | 35.772 | 39.048 | 30.032 | 1.00 | 40.47 | 8 |
| 40 | ATOM | 2408 | N | GLU | B | 96 | 35.663 | 37.637 | 31.765 | 1.00 | 39.61 | 7 |
| | ATOM | 2409 | CA | GLU | B | 96 | 37.020 | 37.175 | 31.582 | 1.00 | 39.82 | 6 |
| | ATOM | 2410 | CB | GLU | B | 96 | 37.765 | 37.046 | 32.915 | 1.00 | 41.36 | 6 |
| | ATOM | 2411 | CG | GLU | B | 96 | 39.238 | 36.644 | 32.763 | 1.00 | 50.17 | 6 |
| | ATOM | 2412 | CD | GLU | B | 96 | 39.989 | 36.540 | 34.094 | 1.00 | 55.05 | 6 |
| 45 | ATOM | 2413 | OE1 | GLU | B | 96 | 39.506 | 37.129 | 35.084 | 1.00 | 57.32 | 8 |
| | ATOM | 2414 | OE2 | GLU | B | 96 | 41.067 | 35.888 | 34.153 | 1.00 | 56.17 | 8 |
| | ATOM | 2415 | C | GLU | B | 96 | 36.802 | 35.804 | 30.966 | 1.00 | 39.55 | 6 |
| | ATOM | 2416 | O | GLU | B | 96 | 36.537 | 34.840 | 31.676 | 1.00 | 38.71 | 8 |
| | ATOM | 2417 | N | VAL | B | 97 | 36.864 | 35.736 | 29.638 | 1.00 | 36.87 | 7 |
| 50 | ATOM | 2418 | CA | VAL | B | 97 | 36.690 | 34.475 | 28.938 | 1.00 | 35.52 | 6 |
| | ATOM | 2419 | CB | VAL | B | 97 | 36.457 | 34.702 | 27.448 | 1.00 | 35.28 | 6 |
| | ATOM | 2420 | CG1 | VAL | B | 97 | 36.249 | 33.378 | 26.752 | 1.00 | 33.50 | 6 |
| | ATOM | 2421 | CG2 | VAL | B | 97 | 35.249 | 35.586 | 27.255 | 1.00 | 31.71 | 6 |
| | ATOM | 2422 | C | VAL | B | 97 | 37.935 | 33.640 | 29.157 | 1.00 | 35.07 | 6 |
| 55 | ATOM | 2423 | O | VAL | B | 97 | 39.025 | 34.005 | 28.741 | 1.00 | 37.13 | 8 |
| | ATOM | 2424 | N | LEU | B | 98 | 37.759 | 32.511 | 29.823 | 1.00 | 35.85 | 7 |
| | ATOM | 2425 | CA | LEU | B | 98 | 38.866 | 31.631 | 30.167 | 1.00 | 36.60 | 6 |
| | ATOM | 2426 | CB | LEU | B | 98 | 38.554 | 30.913 | 31.482 | 1.00 | 37.34 | 6 |
| | ATOM | 2427 | CG | LEU | B | 98 | 38.127 | 31.727 | 32.701 | 1.00 | 39.09 | 6 |
| 60 | ATOM | 2428 | CD1 | LEU | B | 98 | 37.534 | 30.812 | 33.739 | 1.00 | 37.97 | 6 |
| | ATOM | 2429 | CD2 | LEU | B | 98 | 39.306 | 32.469 | 33.259 | 1.00 | 41.28 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2430 | C | LEU | B | 98 | 39.198 | 30.581 | 29.128 | 1.00 | 36.56 | 6 |
| | ATOM | 2431 | O | LEU | B | 98 | 40.195 | 29.889 | 29.251 | 1.00 | 37.06 | 8 |
| | ATOM | 2432 | N | THR | B | 99 | 38.371 | 30.467 | 28.103 | 1.00 | 36.66 | 7 |
| | ATOM | 2433 | CA | THR | B | 99 | 38.578 | 29.438 | 27.100 | 1.00 | 37.03 | 6 |
| 5 | ATOM | 2434 | CB | THR | B | 99 | 37.405 | 28.414 | 27.142 | 1.00 | 40.73 | 6 |
| | ATOM | 2435 | OG1 | THR | B | 99 | 36.152 | 29.097 | 26.972 | 1.00 | 42.70 | 8 |
| | ATOM | 2436 | CG2 | THR | B | 99 | 37.400 | 27.676 | 28.466 | 1.00 | 37.60 | 6 |
| | ATOM | 2437 | C | THR | B | 99 | 38.725 | 29.932 | 25.680 | 1.00 | 34.89 | 6 |
| | ATOM | 2438 | O | THR | B | 99 | 38.401 | 31.073 | 25.378 | 1.00 | 35.25 | 8 |
| 10 | ATOM | 2439 | N | PRO | B | 100 | 39.231 | 29.066 | 24.786 | 1.00 | 35.40 | 7 |
| | ATOM | 2440 | CD | PRO | B | 100 | 39.818 | 27.745 | 25.056 | 1.00 | 33.38 | 6 |
| | ATOM | 2441 | CA | PRO | B | 100 | 39.413 | 29.420 | 23.380 | 1.00 | 35.17 | 6 |
| | ATOM | 2442 | CB | PRO | B | 100 | 39.783 | 28.095 | 22.745 | 1.00 | 33.58 | 6 |
| | ATOM | 2443 | CG | PRO | B | 100 | 40.603 | 27.476 | 23.789 | 1.00 | 34.20 | 6 |
| 15 | ATOM | 2444 | C | PRO | B | 100 | 38.107 | 29.961 | 22.852 | 1.00 | 37.17 | 6 |
| | ATOM | 2445 | O | PRO | B | 100 | 37.052 | 29.396 | 23.103 | 1.00 | 38.59 | 8 |
| | ATOM | 2446 | N | GLN | B | 101 | 38.168 | 31.066 | 22.130 | 1.00 | 39.08 | 7 |
| | ATOM | 2447 | CA | GLN | B | 101 | 36.949 | 31.636 | 21.621 | 1.00 | 40.23 | 6 |
| | ATOM | 2448 | CB | GLN | B | 101 | 37.071 | 33.155 | 21.576 | 1.00 | 39.84 | 6 |
| 20 | ATOM | 2449 | CG | GLN | B | 101 | 36.866 | 33.742 | 22.960 | 1.00 | 45.68 | 6 |
| | ATOM | 2450 | CD | GLN | B | 101 | 37.334 | 35.158 | 23.075 | 1.00 | 47.02 | 6 |
| | ATOM | 2451 | OE1 | GLN | B | 101 | 36.871 | 36.035 | 22.350 | 1.00 | 50.05 | 8 |
| | ATOM | 2452 | NE2 | GLN | B | 101 | 38.260 | 35.398 | 23.997 | 1.00 | 45.46 | 7 |
| | ATOM | 2453 | C | GLN | B | 101 | 36.536 | 31.057 | 20.295 | 1.00 | 39.08 | 6 |
| 25 | ATOM | 2454 | O | GLN | B | 101 | 36.496 | 31.747 | 19.282 | 1.00 | 37.88 | 8 |
| | ATOM | 2455 | N | LEU | B | 102 | 36.212 | 29.768 | 20.342 | 1.00 | 40.24 | 7 |
| | ATOM | 2456 | CA | LEU | B | 102 | 35.770 | 28.997 | 19.183 | 1.00 | 39.64 | 6 |
| | ATOM | 2457 | CB | LEU | B | 102 | 36.652 | 27.759 | 18.982 | 1.00 | 37.23 | 6 |
| | ATOM | 2458 | CG | LEU | B | 102 | 38.155 | 27.988 | 18.842 | 1.00 | 37.24 | 6 |
| 30 | ATOM | 2459 | CD1 | LEU | B | 102 | 38.852 | 26.666 | 18.659 | 1.00 | 33.59 | 6 |
| | ATOM | 2460 | CD2 | LEU | B | 102 | 38.429 | 28.893 | 17.665 | 1.00 | 36.66 | 6 |
| | ATOM | 2461 | C | LEU | B | 102 | 34.349 | 28.528 | 19.394 | 1.00 | 39.73 | 6 |
| | ATOM | 2462 | O | LEU | B | 102 | 33.948 | 28.210 | 20.502 | 1.00 | 38.45 | 8 |
| | ATOM | 2463 | N | ALA | B | 103 | 33.586 | 28.492 | 18.317 | 1.00 | 41.12 | 7 |
| 35 | ATOM | 2464 | CA | ALA | B | 103 | 32.218 | 28.017 | 18.375 | 1.00 | 40.48 | 6 |
| | ATOM | 2465 | CB | ALA | B | 103 | 31.271 | 29.034 | 17.760 | 1.00 | 39.15 | 6 |
| | ATOM | 2466 | C | ALA | B | 103 | 32.163 | 26.711 | 17.599 | 1.00 | 40.28 | 6 |
| | ATOM | 2467 | O | ALA | B | 103 | 33.109 | 26.337 | 16.917 | 1.00 | 38.52 | 8 |
| | ATOM | 2468 | N | ARG | B | 104 | 31.045 | 26.014 | 17.715 | 1.00 | 42.85 | 7 |
| 40 | ATOM | 2469 | CA | ARG | B | 104 | 30.876 | 24.755 | 17.019 | 1.00 | 44.21 | 6 |
| | ATOM | 2470 | CB | ARG | B | 104 | 30.557 | 23.659 | 18.027 | 1.00 | 43.23 | 6 |
| | ATOM | 2471 | CG | ARG | B | 104 | 30.760 | 22.273 | 17.496 | 1.00 | 45.99 | 6 |
| | ATOM | 2472 | CD | ARG | B | 104 | 32.214 | 21.957 | 17.217 | 1.00 | 44.48 | 6 |
| | ATOM | 2473 | NE | ARG | B | 104 | 32.306 | 20.612 | 16.652 | 1.00 | 45.67 | 7 |
| 45 | ATOM | 2474 | CZ | ARG | B | 104 | 33.434 | 19.985 | 16.341 | 1.00 | 42.29 | 6 |
| | ATOM | 2475 | NH1 | ARG | B | 104 | 34.593 | 20.576 | 16.534 | 1.00 | 40.18 | 7 |
| | ATOM | 2476 | NH2 | ARG | B | 104 | 33.397 | 18.755 | 15.847 | 1.00 | 43.70 | 7 |
| | ATOM | 2477 | C | ARG | B | 104 | 29.736 | 24.954 | 16.040 | 1.00 | 44.71 | 6 |
| | ATOM | 2478 | O | ARG | B | 104 | 28.655 | 25.377 | 16.425 | 1.00 | 43.84 | 8 |
| 50 | ATOM | 2479 | N | VAL | B | 105 | 29.990 | 24.686 | 14.767 | 1.00 | 45.98 | 7 |
| | ATOM | 2480 | CA | VAL | B | 105 | 28.955 | 24.862 | 13.761 | 1.00 | 46.86 | 6 |
| | ATOM | 2481 | CB | VAL | B | 105 | 29.404 | 25.834 | 12.663 | 1.00 | 43.67 | 6 |
| | ATOM | 2482 | CG1 | VAL | B | 105 | 28.257 | 26.111 | 11.715 | 1.00 | 42.93 | 6 |
| | ATOM | 2483 | CG2 | VAL | B | 105 | 29.885 | 27.116 | 13.281 | 1.00 | 41.79 | 6 |
| 55 | ATOM | 2484 | C | VAL | B | 105 | 28.546 | 23.546 | 13.112 | 1.00 | 50.58 | 6 |
| | ATOM | 2485 | O | VAL | B | 105 | 29.393 | 22.808 | 12.589 | 1.00 | 51.09 | 8 |
| | ATOM | 2486 | N | VAL | B | 106 | 27.243 | 23.266 | 13.158 | 1.00 | 51.24 | 7 |
| | ATOM | 2487 | CA | VAL | B | 106 | 26.677 | 22.056 | 12.577 | 1.00 | 52.00 | 6 |
| | ATOM | 2488 | CB | VAL | B | 106 | 25.464 | 21.592 | 13.387 | 1.00 | 52.31 | 6 |
| 60 | ATOM | 2489 | CG1 | VAL | B | 106 | 25.038 | 20.207 | 12.931 | 1.00 | 52.15 | 6 |
| | ATOM | 2490 | CG2 | VAL | B | 106 | 25.798 | 21.607 | 14.865 | 1.00 | 50.55 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 2491 | C | VAL | B | 106 | 26.243 | 22.369 | 11.147 | 1.00 | 52.00 | 6 |
| | ATOM | 2492 | O | VAL | B | 106 | 25.782 | 23.474 | 10.870 | 1.00 | 52.80 | 8 |
| | ATOM | 2493 | N | SER | B | 107 | 26.388 | 21.401 | 10.248 | 1.00 | 51.28 | 7 |
| | ATOM | 2494 | CA | SER | B | 107 | 26.038 | 21.592 | 8.845 | 1.00 | 52.41 | 6 |
| 5 | ATOM | 2495 | CB | SER | B | 107 | 26.175 | 20.272 | 8.097 | 1.00 | 54.05 | 6 |
| | ATOM | 2496 | OG | SER | B | 107 | 25.609 | 19.216 | 8.855 | 1.00 | 58.60 | 8 |
| | ATOM | 2497 | C | SER | B | 107 | 24.676 | 22.198 | 8.544 | 1.00 | 52.33 | 6 |
| | ATOM | 2498 | O | SER | B | 107 | 24.469 | 22.728 | 7.460 | 1.00 | 52.31 | 8 |
| | ATOM | 2499 | N | ASP | B | 108 | 23.753 | 22.132 | 9.494 | 1.00 | 54.48 | 7 |
| 10 | ATOM | 2500 | CA | ASP | B | 108 | 22.417 | 22.687 | 9.285 | 1.00 | 57.36 | 6 |
| | ATOM | 2501 | CB | ASP | B | 108 | 21.376 | 21.830 | 10.007 | 1.00 | 59.13 | 6 |
| | ATOM | 2502 | CG | ASP | B | 108 | 21.474 | 21.933 | 11.512 | 1.00 | 61.77 | 6 |
| | ATOM | 2503 | OD1 | ASP | B | 108 | 22.604 | 21.993 | 12.034 | 1.00 | 63.26 | 8 |
| | ATOM | 2504 | OD2 | ASP | B | 108 | 20.419 | 21.941 | 12.180 | 1.00 | 63.13 | 8 |
| 15 | ATOM | 2505 | C | ASP | B | 108 | 22.266 | 24.152 | 9.715 | 1.00 | 58.76 | 6 |
| | ATOM | 2506 | O | ASP | B | 108 | 21.163 | 24.696 | 9.711 | 1.00 | 60.28 | 8 |
| | ATOM | 2507 | N | GLY | B | 109 | 23.376 | 24.784 | 10.087 | 1.00 | 59.97 | 7 |
| | ATOM | 2508 | CA | GLY | B | 109 | 23.346 | 26.175 | 10.489 | 1.00 | 58.62 | 6 |
| | ATOM | 2509 | C | GLY | B | 109 | 23.213 | 26.394 | 11.983 | 1.00 | 59.08 | 6 |
| 20 | ATOM | 2510 | O | GLY | B | 109 | 23.123 | 27.534 | 12.437 | 1.00 | 58.71 | 8 |
| | ATOM | 2511 | N | GLU | B | 110 | 23.187 | 25.317 | 12.758 | 1.00 | 58.29 | 7 |
| | ATOM | 2512 | CA | GLU | B | 110 | 23.062 | 25.451 | 14.202 | 1.00 | 57.49 | 6 |
| | ATOM | 2513 | CB | GLU | B | 110 | 22.619 | 24.125 | 14.827 | 1.00 | 60.94 | 6 |
| | ATOM | 2514 | CG | GLU | B | 110 | 21.947 | 24.234 | 16.208 | 1.00 | 64.96 | 6 |
| 25 | ATOM | 2515 | CD | GLU | B | 110 | 20.623 | 25.007 | 16.159 | 1.00 | 69.09 | 6 |
| | ATOM | 2516 | OE1 | GLU | B | 110 | 20.054 | 25.121 | 15.044 | 1.00 | 70.48 | 8 |
| | ATOM | 2517 | OE2 | GLU | B | 110 | 20.146 | 25.493 | 17.223 | 1.00 | 67.90 | 8 |
| | ATOM | 2518 | C | GLU | B | 110 | 24.432 | 25.838 | 14.723 | 1.00 | 56.48 | 6 |
| | ATOM | 2519 | O | GLU | B | 110 | 25.447 | 25.291 | 14.282 | 1.00 | 58.51 | 8 |
| 30 | ATOM | 2520 | N | VAL | B | 111 | 24.461 | 26.780 | 15.656 | 1.00 | 52.94 | 7 |
| | ATOM | 2521 | CA | VAL | B | 111 | 25.706 | 27.254 | 16.237 | 1.00 | 49.98 | 6 |
| | ATOM | 2522 | CB | VAL | B | 111 | 25.933 | 28.743 | 15.914 | 1.00 | 50.06 | 6 |
| | ATOM | 2523 | CG1 | VAL | B | 111 | 27.259 | 29.199 | 16.502 | 1.00 | 48.91 | 6 |
| | ATOM | 2524 | CG2 | VAL | B | 111 | 25.894 | 28.973 | 14.406 | 1.00 | 49.75 | 6 |
| 35 | ATOM | 2525 | C | VAL | B | 111 | 25.702 | 27.095 | 17.749 | 1.00 | 49.14 | 6 |
| | ATOM | 2526 | O | VAL | B | 111 | 24.730 | 27.431 | 18.413 | 1.00 | 47.85 | 8 |
| | ATOM | 2527 | N | LEU | B | 112 | 26.795 | 26.581 | 18.292 | 1.00 | 49.78 | 7 |
| | ATOM | 2528 | CA | LEU | B | 112 | 26.907 | 26.404 | 19.733 | 1.00 | 50.84 | 6 |
| | ATOM | 2529 | CB | LEU | B | 112 | 26.903 | 24.914 | 20.107 | 1.00 | 54.21 | 6 |
| 40 | ATOM | 2530 | CG | LEU | B | 112 | 26.075 | 23.868 | 19.337 | 1.00 | 56.22 | 6 |
| | ATOM | 2531 | CD1 | LEU | B | 112 | 24.673 | 24.393 | 19.025 | 1.00 | 58.51 | 6 |
| | ATOM | 2532 | CD2 | LEU | B | 112 | 26.802 | 23.504 | 18.065 | 1.00 | 54.95 | 6 |
| | ATOM | 2533 | C | LEU | B | 112 | 28.202 | 27.038 | 20.242 | 1.00 | 50.58 | 6 |
| | ATOM | 2534 | O | LEU | B | 112 | 29.300 | 26.651 | 19.829 | 1.00 | 51.33 | 8 |
| 45 | ATOM | 2535 | N | TYR | B | 113 | 28.073 | 28.013 | 21.134 | 1.00 | 47.63 | 7 |
| | ATOM | 2536 | CA | TYR | B | 113 | 29.227 | 28.681 | 21.709 | 1.00 | 46.01 | 6 |
| | ATOM | 2537 | CB | TYR | B | 113 | 29.266 | 30.154 | 21.279 | 1.00 | 45.50 | 6 |
| | ATOM | 2538 | CG | TYR | B | 113 | 30.415 | 30.970 | 21.868 | 1.00 | 45.48 | 6 |
| | ATOM | 2539 | CD1 | TYR | B | 113 | 31.715 | 30.468 | 21.902 | 1.00 | 43.49 | 6 |
| 50 | ATOM | 2540 | CE1 | TYR | B | 113 | 32.766 | 31.225 | 22.412 | 1.00 | 42.81 | 6 |
| | ATOM | 2541 | CD2 | TYR | B | 113 | 30.200 | 32.262 | 22.367 | 1.00 | 44.88 | 6 |
| | ATOM | 2542 | CE2 | TYR | B | 113 | 31.246 | 33.022 | 22.876 | 1.00 | 42.75 | 6 |
| | ATOM | 2543 | CZ | TYR | B | 113 | 32.528 | 32.499 | 22.897 | 1.00 | 45.11 | 6 |
| | ATOM | 2544 | OH | TYR | B | 113 | 33.579 | 33.248 | 23.397 | 1.00 | 46.12 | 8 |
| 55 | ATOM | 2545 | C | TYR | B | 113 | 29.081 | 28.561 | 23.208 | 1.00 | 45.62 | 6 |
| | ATOM | 2546 | O | TYR | B | 113 | 28.130 | 29.064 | 23.783 | 1.00 | 48.17 | 8 |
| | ATOM | 2547 | N | MET | B | 114 | 30.025 | 27.887 | 23.842 | 1.00 | 45.82 | 7 |
| | ATOM | 2548 | CA | MET | B | 114 | 29.966 | 27.691 | 25.280 | 1.00 | 47.40 | 6 |
| | ATOM | 2549 | CB | MET | B | 114 | 29.652 | 26.237 | 25.578 | 1.00 | 51.46 | 6 |
| 60 | ATOM | 2550 | CG | MET | B | 114 | 29.408 | 25.958 | 27.030 | 1.00 | 56.47 | 6 |
| | ATOM | 2551 | SD | MET | B | 114 | 29.463 | 24.204 | 27.290 | 1.00 | 61.08 | 16 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2552 | CE | MET | B | 114 | 27.833 | 23.732 | 26.736 | 1.00 | 59.81 | 6 |
| | ATOM | 2553 | C | MET | B | 114 | 31.281 | 28.060 | 25.944 | 1.00 | 47.40 | 6 |
| | ATOM | 2554 | O | MET | B | 114 | 32.093 | 27.187 | 26.268 | 1.00 | 46.46 | 8 |
| | ATOM | 2555 | N | PRO | B | 115 | 31.511 | 29.364 | 26.158 | 1.00 | 46.76 | 7 |
| 5 | ATOM | 2556 | CD | PRO | B | 115 | 30.680 | 30.502 | 25.712 | 1.00 | 45.52 | 6 |
| | ATOM | 2557 | CA | PRO | B | 115 | 32.744 | 29.832 | 26.786 | 1.00 | 44.75 | 6 |
| | ATOM | 2558 | CB | PRO | B | 115 | 32.834 | 31.259 | 26.285 | 1.00 | 47.19 | 6 |
| | ATOM | 2559 | CG | PRO | B | 115 | 31.382 | 31.687 | 26.316 | 1.00 | 45.23 | 6 |
| | ATOM | 2560 | C | PRO | B | 115 | 32.653 | 29.776 | 28.303 | 1.00 | 45.76 | 6 |
| 10 | ATOM | 2561 | O | PRO | B | 115 | 31.567 | 29.933 | 28.865 | 1.00 | 46.79 | 8 |
| | ATOM | 2562 | N | SER | B | 116 | 33.783 | 29.545 | 28.965 | 1.00 | 44.58 | 7 |
| | ATOM | 2563 | CA | SER | B | 116 | 33.797 | 29.527 | 30.416 | 1.00 | 42.97 | 6 |
| | ATOM | 2564 | CB | SER | B | 116 | 34.867 | 28.605 | 30.935 | 1.00 | 42.63 | 6 |
| | ATOM | 2565 | OG | SER | B | 116 | 34.810 | 28.586 | 32.342 | 1.00 | 46.80 | 8 |
| 15 | ATOM | 2566 | C | SER | B | 116 | 34.124 | 30.939 | 30.832 | 1.00 | 43.61 | 6 |
| | ATOM | 2567 | O | SER | B | 116 | 35.144 | 31.473 | 30.431 | 1.00 | 45.91 | 8 |
| | ATOM | 2568 | N | ILE | B | 117 | 33.270 | 31.547 | 31.643 | 1.00 | 42.76 | 7 |
| | ATOM | 2569 | CA | ILE | B | 117 | 33.483 | 32.923 | 32.052 | 1.00 | 40.88 | 6 |
| | ATOM | 2570 | CB | ILE | B | 117 | 32.340 | 33.816 | 31.515 | 1.00 | 39.30 | 6 |
| 20 | ATOM | 2571 | CG2 | ILE | B | 117 | 32.512 | 35.249 | 31.995 | 1.00 | 40.17 | 6 |
| | ATOM | 2572 | CG1 | ILE | B | 117 | 32.317 | 33.760 | 29.992 | 1.00 | 37.44 | 6 |
| | ATOM | 2573 | CD1 | ILE | B | 117 | 31.069 | 34.332 | 29.394 | 1.00 | 36.96 | 6 |
| | ATOM | 2574 | C | ILE | B | 117 | 33.592 | 33.158 | 33.545 | 1.00 | 42.01 | 6 |
| | ATOM | 2575 | O | ILE | B | 117 | 32.840 | 32.585 | 34.329 | 1.00 | 44.14 | 8 |
| 25 | ATOM | 2576 | N | ARG | B | 118 | 34.554 | 33.986 | 33.939 | 1.00 | 42.44 | 7 |
| | ATOM | 2577 | CA | ARG | B | 118 | 34.683 | 34.363 | 35.339 | 1.00 | 42.12 | 6 |
| | ATOM | 2578 | CB | ARG | B | 118 | 36.120 | 34.283 | 35.835 | 1.00 | 39.55 | 6 |
| | ATOM | 2579 | CG | ARG | B | 118 | 36.241 | 34.873 | 37.226 | 1.00 | 40.13 | 6 |
| | ATOM | 2580 | CD | ARG | B | 118 | 37.520 | 34.517 | 37.933 | 1.00 | 40.72 | 6 |
| 30 | ATOM | 2581 | NE | ARG | B | 118 | 37.546 | 35.120 | 39.259 | 1.00 | 43.73 | 7 |
| | ATOM | 2582 | CZ | ARG | B | 118 | 38.424 | 34.821 | 40.204 | 1.00 | 43.99 | 6 |
| | ATOM | 2583 | NH1 | ARG | B | 118 | 39.356 | 33.915 | 39.973 | 1.00 | 45.99 | 7 |
| | ATOM | 2584 | NH2 | ARG | B | 118 | 38.367 | 35.427 | 41.376 | 1.00 | 44.09 | 7 |
| | ATOM | 2585 | C | ARG | B | 118 | 34.215 | 35.819 | 35.332 | 1.00 | 42.68 | 6 |
| 35 | ATOM | 2586 | O | ARG | B | 118 | 34.657 | 36.604 | 34.503 | 1.00 | 43.76 | 8 |
| | ATOM | 2587 | N | GLN | B | 119 | 33.324 | 36.190 | 36.239 | 1.00 | 41.50 | 7 |
| | ATOM | 2588 | CA | GLN | B | 119 | 32.815 | 37.553 | 36.229 | 1.00 | 40.73 | 6 |
| | ATOM | 2589 | CB | GLN | B | 119 | 31.817 | 37.664 | 35.080 | 1.00 | 37.47 | 6 |
| | ATOM | 2590 | CG | GLN | B | 119 | 31.199 | 39.002 | 34.850 | 1.00 | 37.63 | 6 |
| 40 | ATOM | 2591 | CD | GLN | B | 119 | 30.414 | 39.031 | 33.553 | 1.00 | 38.05 | 6 |
| | ATOM | 2592 | OE1 | GLN | B | 119 | 29.835 | 38.028 | 33.137 | 1.00 | 40.82 | 8 |
| | ATOM | 2593 | NE2 | GLN | B | 119 | 30.380 | 40.181 | 32.914 | 1.00 | 38.24 | 7 |
| | ATOM | 2594 | C | GLN | B | 119 | 32.171 | 37.897 | 37.561 | 1.00 | 41.65 | 6 |
| | ATOM | 2595 | O | GLN | B | 119 | 31.660 | 37.028 | 38.245 | 1.00 | 43.20 | 8 |
| 45 | ATOM | 2596 | N | ARG | B | 120 | 32.208 | 39.163 | 37.945 | 1.00 | 43.19 | 7 |
| | ATOM | 2597 | CA | ARG | B | 120 | 31.606 | 39.561 | 39.209 | 1.00 | 46.59 | 6 |
| | ATOM | 2598 | CB | ARG | B | 120 | 32.500 | 40.540 | 39.955 | 1.00 | 48.44 | 6 |
| | ATOM | 2599 | CG | ARG | B | 120 | 33.874 | 40.005 | 40.232 | 1.00 | 57.79 | 6 |
| | ATOM | 2600 | CD | ARG | B | 120 | 34.423 | 40.632 | 41.493 | 1.00 | 64.95 | 6 |
| 50 | ATOM | 2601 | NE | ARG | B | 120 | 33.964 | 39.971 | 42.727 | 1.00 | 67.80 | 7 |
| | ATOM | 2602 | CZ | ARG | B | 120 | 33.571 | 40.624 | 43.818 | 1.00 | 68.76 | 6 |
| | ATOM | 2603 | NH1 | ARG | B | 120 | 33.565 | 41.958 | 43.827 | 1.00 | 66.34 | 7 |
| | ATOM | 2604 | NH2 | ARG | B | 120 | 33.219 | 39.944 | 44.913 | 1.00 | 69.34 | 7 |
| | ATOM | 2605 | C | ARG | B | 120 | 30.241 | 40.184 | 38.999 | 1.00 | 45.42 | 6 |
| 55 | ATOM | 2606 | O | ARG | B | 120 | 29.991 | 40.825 | 37.979 | 1.00 | 43.82 | 8 |
| | ATOM | 2607 | N | PHE | B | 121 | 29.361 | 39.983 | 39.972 | 1.00 | 45.27 | 7 |
| | ATOM | 2608 | CA | PHE | B | 121 | 28.012 | 40.515 | 39.882 | 1.00 | 46.73 | 6 |
| | ATOM | 2609 | CB | PHE | B | 121 | 26.998 | 39.411 | 39.558 | 1.00 | 44.66 | 6 |
| | ATOM | 2610 | CG | PHE | B | 121 | 27.320 | 38.639 | 38.324 | 1.00 | 41.56 | 6 |
| 60 | ATOM | 2611 | CD1 | PHE | B | 121 | 28.265 | 37.621 | 38.355 | 1.00 | 38.98 | 6 |
| | ATOM | 2612 | CD2 | PHE | B | 121 | 26.698 | 38.942 | 37.123 | 1.00 | 40.65 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 2613 | CE1 | PHE | B | 121 | 28.585 | 36.920 | 37.212 | 1.00 | 38.44 | 6 |
| | ATOM | 2614 | CE2 | PHE | B | 121 | 27.013 | 38.245 | 35.977 | 1.00 | 38.36 | 6 |
| | ATOM | 2615 | CZ | PHE | B | 121 | 27.959 | 37.232 | 36.020 | 1.00 | 37.80 | 6 |
| 5 | ATOM | 2616 | C | PHE | B | 121 | 27.549 | 41.193 | 41.142 | 1.00 | 47.76 | 6 |
| | ATOM | 2617 | O | PHE | B | 121 | 28.094 | 40.972 | 42.224 | 1.00 | 45.87 | 8 |
| | ATOM | 2618 | N | SER | B | 122 | 26.521 | 42.021 | 40.966 | 1.00 | 49.39 | 7 |
| | ATOM | 2619 | CA | SER | B | 122 | 25.881 | 42.735 | 42.054 | 1.00 | 51.30 | 6 |
| | ATOM | 2620 | CB | SER | B | 122 | 25.677 | 44.200 | 41.680 | 1.00 | 50.63 | 6 |
| 10 | ATOM | 2621 | OG | SER | B | 122 | 25.026 | 44.887 | 42.726 | 1.00 | 52.75 | 8 |
| | ATOM | 2622 | C | SER | B | 122 | 24.530 | 42.041 | 42.235 | 1.00 | 52.14 | 6 |
| | ATOM | 2623 | O | SER | B | 122 | 23.659 | 42.135 | 41.377 | 1.00 | 51.12 | 8 |
| | ATOM | 2624 | N | CYS | B | 123 | 24.371 | 41.323 | 43.340 | 1.00 | 53.84 | 7 |
| | ATOM | 2625 | CA | CYS | B | 123 | 23.133 | 40.605 | 43.603 | 1.00 | 56.99 | 6 |
| 15 | ATOM | 2626 | C | CYS | B | 123 | 22.973 | 40.343 | 45.111 | 1.00 | 58.94 | 6 |
| | ATOM | 2627 | O | CYS | B | 123 | 23.837 | 40.727 | 45.911 | 1.00 | 58.00 | 8 |
| | ATOM | 2628 | CB | CYS | B | 123 | 23.135 | 39.282 | 42.830 | 1.00 | 55.83 | 6 |
| | ATOM | 2629 | SG | CYS | B | 123 | 24.561 | 38.231 | 43.250 | 1.00 | 57.55 | 16 |
| | ATOM | 2630 | N | ASP | B | 124 | 21.874 | 39.687 | 45.491 | 1.00 | 59.24 | 7 |
| 20 | ATOM | 2631 | CA | ASP | B | 124 | 21.619 | 39.412 | 46.893 | 1.00 | 59.17 | 6 |
| | ATOM | 2632 | CB | ASP | B | 124 | 20.148 | 39.085 | 47.114 | 1.00 | 61.47 | 6 |
| | ATOM | 2633 | CG | ASP | B | 124 | 19.670 | 39.487 | 48.505 | 1.00 | 62.03 | 6 |
| | ATOM | 2634 | OD1 | ASP | B | 124 | 20.462 | 39.403 | 49.470 | 1.00 | 60.72 | 8 |
| | ATOM | 2635 | OD2 | ASP | B | 124 | 18.493 | 39.886 | 48.628 | 1.00 | 63.80 | 8 |
| 25 | ATOM | 2636 | C | ASP | B | 124 | 22.470 | 38.274 | 47.434 | 1.00 | 59.25 | 6 |
| | ATOM | 2637 | O | ASP | B | 124 | 22.309 | 37.122 | 47.036 | 1.00 | 58.84 | 8 |
| | ATOM | 2638 | N | VAL | B | 125 | 23.365 | 38.612 | 48.356 | 1.00 | 59.36 | 7 |
| | ATOM | 2639 | CA | VAL | B | 125 | 24.260 | 37.647 | 48.979 | 1.00 | 59.62 | 6 |
| | ATOM | 2640 | CB | VAL | B | 125 | 25.683 | 38.230 | 49.080 | 1.00 | 57.35 | 6 |
| 30 | ATOM | 2641 | CG1 | VAL | B | 125 | 26.599 | 37.280 | 49.798 | 1.00 | 54.50 | 6 |
| | ATOM | 2642 | CG2 | VAL | B | 125 | 26.212 | 38.519 | 47.702 | 1.00 | 58.35 | 6 |
| | ATOM | 2643 | C | VAL | B | 125 | 23.766 | 37.277 | 50.378 | 1.00 | 62.42 | 6 |
| | ATOM | 2644 | O | VAL | B | 125 | 24.161 | 36.254 | 50.938 | 1.00 | 64.51 | 8 |
| | ATOM | 2645 | N | SER | B | 126 | 22.892 | 38.105 | 50.939 | 1.00 | 63.61 | 7 |
| 35 | ATOM | 2646 | CA | SER | B | 126 | 22.375 | 37.857 | 52.283 | 1.00 | 64.32 | 6 |
| | ATOM | 2647 | CB | SER | B | 126 | 21.260 | 38.857 | 52.613 | 1.00 | 63.21 | 6 |
| | ATOM | 2648 | OG | SER | B | 126 | 20.175 | 38.715 | 51.715 | 1.00 | 59.22 | 8 |
| | ATOM | 2649 | C | SER | B | 126 | 21.858 | 36.429 | 52.444 | 1.00 | 64.47 | 6 |
| | ATOM | 2650 | O | SER | B | 126 | 21.082 | 35.940 | 51.626 | 1.00 | 63.31 | 8 |
| 40 | ATOM | 2651 | N | GLY | B | 127 | 22.313 | 35.764 | 53.496 | 1.00 | 65.55 | 7 |
| | ATOM | 2652 | CA | GLY | B | 127 | 21.872 | 34.409 | 53.748 | 1.00 | 68.84 | 6 |
| | ATOM | 2653 | C | GLY | B | 127 | 22.847 | 33.351 | 53.282 | 1.00 | 70.32 | 6 |
| | ATOM | 2654 | O | GLY | B | 127 | 22.634 | 32.161 | 53.500 | 1.00 | 71.17 | 8 |
| | ATOM | 2655 | N | VAL | B | 128 | 23.923 | 33.776 | 52.638 | 1.00 | 71.67 | 7 |
| 45 | ATOM | 2656 | CA | VAL | B | 128 | 24.910 | 32.826 | 52.148 | 1.00 | 72.95 | 6 |
| | ATOM | 2657 | CB | VAL | B | 128 | 26.107 | 33.522 | 51.467 | 1.00 | 71.97 | 6 |
| | ATOM | 2658 | CG1 | VAL | B | 128 | 25.686 | 34.081 | 50.149 | 1.00 | 73.72 | 6 |
| | ATOM | 2659 | CG2 | VAL | B | 128 | 26.654 | 34.614 | 52.359 | 1.00 | 69.90 | 6 |
| | ATOM | 2660 | C | VAL | B | 128 | 25.504 | 31.942 | 53.212 | 1.00 | 73.83 | 6 |
| 50 | ATOM | 2661 | O | VAL | B | 128 | 25.628 | 30.743 | 53.016 | 1.00 | 73.27 | 8 |
| | ATOM | 2662 | N | ASP | B | 129 | 25.884 | 32.542 | 54.332 | 1.00 | 75.83 | 7 |
| | ATOM | 2663 | CA | ASP | B | 129 | 26.532 | 31.789 | 55.384 | 1.00 | 78.34 | 6 |
| | ATOM | 2664 | CB | ASP | B | 129 | 27.008 | 32.715 | 56.504 | 1.00 | 79.36 | 6 |
| | ATOM | 2665 | CG | ASP | B | 129 | 28.209 | 32.141 | 57.257 | 1.00 | 81.22 | 6 |
| 55 | ATOM | 2666 | OD1 | ASP | B | 129 | 29.166 | 32.909 | 57.523 | 1.00 | 81.78 | 8 |
| | ATOM | 2667 | OD2 | ASP | B | 129 | 28.202 | 30.922 | 57.576 | 1.00 | 81.70 | 8 |
| | ATOM | 2668 | C | ASP | B | 129 | 25.720 | 30.648 | 55.972 | 1.00 | 80.31 | 6 |
| | ATOM | 2669 | O | ASP | B | 129 | 26.293 | 29.783 | 56.660 | 1.00 | 81.06 | 8 |
| | ATOM | 2670 | N | THR | B | 130 | 24.412 | 30.603 | 55.706 | 1.00 | 80.80 | 7 |
| 60 | ATOM | 2671 | CA | THR | B | 130 | 23.640 | 29.501 | 56.259 | 1.00 | 81.78 | 6 |
| | ATOM | 2672 | CB | THR | B | 130 | 23.681 | 29.563 | 57.799 | 1.00 | 85.11 | 6 |
| | ATOM | 2673 | OG1 | THR | B | 130 | 24.158 | 30.862 | 58.195 | 1.00 | 84.93 | 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 2674 | CG2 | THR | B | 130 | 24.582 | 28.416 | 58.388 | 1.00 | 85.83 | 6 |
| | ATOM | 2675 | C | THR | B | 130 | 22.182 | 29.286 | 55.881 | 1.00 | 80.84 | 6 |
| | ATOM | 2676 | O | THR | B | 130 | 21.460 | 30.224 | 55.506 | 1.00 | 78.93 | 8 |
| | ATOM | 2677 | N | GLU | B | 131 | 21.784 | 28.014 | 56.028 | 1.00 | 80.92 | 7 |
| 5 | ATOM | 2678 | CA | GLU | B | 131 | 20.416 | 27.510 | 55.832 | 1.00 | 80.70 | 6 |
| | ATOM | 2679 | CB | GLU | B | 131 | 19.435 | 28.339 | 56.689 | 1.00 | 83.05 | 6 |
| | ATOM | 2680 | CG | GLU | B | 131 | 19.467 | 28.017 | 58.187 | 1.00 | 84.49 | 6 |
| | ATOM | 2681 | CD | GLU | B | 131 | 19.024 | 29.189 | 59.051 | 1.00 | 85.34 | 6 |
| | ATOM | 2682 | OE1 | GLU | B | 131 | 17.948 | 29.773 | 58.762 | 1.00 | 86.44 | 8 |
| 10 | ATOM | 2683 | OE2 | GLU | B | 131 | 19.757 | 29.521 | 60.019 | 1.00 | 85.14 | 8 |
| | ATOM | 2684 | C | GLU | B | 131 | 19.864 | 27.420 | 54.426 | 1.00 | 79.07 | 6 |
| | ATOM | 2685 | O | GLU | B | 131 | 20.207 | 26.520 | 53.643 | 1.00 | 76.96 | 8 |
| | ATOM | 2686 | N | SER | B | 132 | 18.941 | 28.338 | 54.156 | 1.00 | 78.17 | 7 |
| | ATOM | 2687 | CA | SER | B | 132 | 18.298 | 28.449 | 52.858 | 1.00 | 77.92 | 6 |
| 15 | ATOM | 2688 | CB | SER | B | 132 | 16.953 | 29.195 | 53.001 | 1.00 | 77.07 | 6 |
| | ATOM | 2689 | OG | SER | B | 132 | 17.130 | 30.486 | 53.575 | 1.00 | 77.45 | 8 |
| | ATOM | 2690 | C | SER | B | 132 | 19.277 | 29.220 | 51.945 | 1.00 | 76.88 | 6 |
| | ATOM | 2691 | O | SER | B | 132 | 19.000 | 29.463 | 50.759 | 1.00 | 77.41 | 8 |
| | ATOM | 2692 | N | GLY | B | 133 | 20.424 | 29.588 | 52.520 | 1.00 | 74.38 | 7 |
| 20 | ATOM | 2693 | CA | GLY | B | 133 | 21.442 | 30.308 | 51.782 | 1.00 | 72.04 | 6 |
| | ATOM | 2694 | C | GLY | B | 133 | 20.943 | 31.569 | 51.105 | 1.00 | 71.42 | 6 |
| | ATOM | 2695 | O | GLY | B | 133 | 19.888 | 32.104 | 51.450 | 1.00 | 71.39 | 8 |
| | ATOM | 2696 | N | ALA | B | 134 | 21.708 | 32.044 | 50.125 | 1.00 | 69.68 | 7 |
| | ATOM | 2697 | CA | ALA | B | 134 | 21.345 | 33.251 | 49.390 | 1.00 | 66.69 | 6 |
| 25 | ATOM | 2698 | CB | ALA | B | 134 | 22.534 | 34.194 | 49.315 | 1.00 | 66.34 | 6 |
| | ATOM | 2699 | C | ALA | B | 134 | 20.874 | 32.908 | 47.993 | 1.00 | 64.53 | 6 |
| | ATOM | 2700 | O | ALA | B | 134 | 21.095 | 31.802 | 47.504 | 1.00 | 64.56 | 8 |
| | ATOM | 2701 | N | THR | B | 135 | 20.207 | 33.865 | 47.369 | 1.00 | 62.63 | 7 |
| | ATOM | 2702 | CA | THR | B | 135 | 19.719 | 33.696 | 46.017 | 1.00 | 62.23 | 6 |
| 30 | ATOM | 2703 | CB | THR | B | 135 | 18.205 | 33.577 | 45.980 | 1.00 | 62.17 | 6 |
| | ATOM | 2704 | OG1 | THR | B | 135 | 17.812 | 32.456 | 46.775 | 1.00 | 64.85 | 8 |
| | ATOM | 2705 | CG2 | THR | B | 135 | 17.721 | 33.370 | 44.543 | 1.00 | 62.33 | 6 |
| | ATOM | 2706 | C | THR | B | 135 | 20.159 | 34.900 | 45.194 | 1.00 | 62.39 | 6 |
| | ATOM | 2707 | O | THR | B | 135 | 19.618 | 36.009 | 45.308 | 1.00 | 62.56 | 8 |
| 35 | ATOM | 2708 | N | CYS | B | 136 | 21.174 | 34.661 | 44.379 | 1.00 | 61.14 | 7 |
| | ATOM | 2709 | CA | CYS | B | 136 | 21.754 | 35.668 | 43.526 | 1.00 | 58.61 | 6 |
| | ATOM | 2710 | C | CYS | B | 136 | 21.159 | 35.497 | 42.134 | 1.00 | 56.85 | 6 |
| | ATOM | 2711 | O | CYS | B | 136 | 21.308 | 34.452 | 41.503 | 1.00 | 55.78 | 8 |
| | ATOM | 2712 | CB | CYS | B | 136 | 23.276 | 35.474 | 43.527 | 1.00 | 58.82 | 6 |
| 40 | ATOM | 2713 | SG | CYS | B | 136 | 24.201 | 36.455 | 42.315 | 1.00 | 60.36 | 16 |
| | ATOM | 2714 | N | ARG | B | 137 | 20.453 | 36.519 | 41.670 | 1.00 | 55.98 | 7 |
| | ATOM | 2715 | CA | ARG | B | 137 | 19.845 | 36.457 | 40.353 | 1.00 | 56.14 | 6 |
| | ATOM | 2716 | CB | ARG | B | 137 | 18.421 | 37.009 | 40.383 | 1.00 | 57.73 | 6 |
| | ATOM | 2717 | CG | ARG | B | 137 | 17.502 | 36.250 | 41.303 | 1.00 | 62.21 | 6 |
| 45 | ATOM | 2718 | CD | ARG | B | 137 | 16.367 | 37.136 | 41.792 | 1.00 | 68.77 | 6 |
| | ATOM | 2719 | NE | ARG | B | 137 | 15.827 | 36.666 | 43.071 | 1.00 | 74.27 | 7 |
| | ATOM | 2720 | CZ | ARG | B | 137 | 15.070 | 35.575 | 43.224 | 1.00 | 76.32 | 6 |
| | ATOM | 2721 | NH1 | ARG | B | 137 | 14.739 | 34.822 | 42.174 | 1.00 | 77.05 | 7 |
| | ATOM | 2722 | NH2 | ARG | B | 137 | 14.652 | 35.221 | 44.434 | 1.00 | 75.79 | 7 |
| 50 | ATOM | 2723 | C | ARG | B | 137 | 20.672 | 37.253 | 39.366 | 1.00 | 55.38 | 6 |
| | ATOM | 2724 | O | ARG | B | 137 | 21.052 | 38.389 | 39.637 | 1.00 | 57.67 | 8 |
| | ATOM | 2725 | N | ILE | B | 138 | 20.933 | 36.646 | 38.215 | 1.00 | 52.27 | 7 |
| | ATOM | 2726 | CA | ILE | B | 138 | 21.716 | 37.255 | 37.163 | 1.00 | 48.96 | 6 |
| | ATOM | 2727 | CB | ILE | B | 138 | 22.977 | 36.411 | 36.890 | 1.00 | 45.32 | 6 |
| 55 | ATOM | 2728 | CG2 | ILE | B | 138 | 23.751 | 37.007 | 35.749 | 1.00 | 42.82 | 6 |
| | ATOM | 2729 | CG1 | ILE | B | 138 | 23.822 | 36.309 | 38.160 | 1.00 | 42.90 | 6 |
| | ATOM | 2730 | CD1 | ILE | B | 138 | 24.931 | 35.313 | 38.067 | 1.00 | 40.32 | 6 |
| | ATOM | 2731 | C | ILE | B | 138 | 20.863 | 37.313 | 35.900 | 1.00 | 48.66 | 6 |
| | ATOM | 2732 | O | ILE | B | 138 | 20.420 | 36.286 | 35.406 | 1.00 | 49.73 | 8 |
| 60 | ATOM | 2733 | N | LYS | B | 139 | 20.628 | 38.506 | 35.375 | 1.00 | 48.12 | 7 |
| | ATOM | 2734 | CA | LYS | B | 139 | 19.822 | 38.642 | 34.165 | 1.00 | 51.18 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2735 | CB | LYS | B | 139 | 18.775 | 39.759 | 34.326 | 1.00 | 52.93 | 6 |
| | ATOM | 2736 | CG | LYS | B | 139 | 17.908 | 39.625 | 35.553 | 1.00 | 56.09 | 6 |
| | ATOM | 2737 | CD | LYS | B | 139 | 16.721 | 40.567 | 35.523 | 1.00 | 58.54 | 6 |
| 5 | ATOM | 2738 | CE | LYS | B | 139 | 15.716 | 40.155 | 34.461 | 1.00 | 59.19 | 6 |
| | ATOM | 2739 | NZ | LYS | B | 139 | 14.539 | 41.062 | 34.435 | 1.00 | 59.74 | 7 |
| | ATOM | 2740 | C | LYS | B | 139 | 20.686 | 38.966 | 32.957 | 1.00 | 50.79 | 6 |
| | ATOM | 2741 | O | LYS | B | 139 | 21.461 | 39.919 | 32.998 | 1.00 | 53.10 | 8 |
| | ATOM | 2742 | N | ILE | B | 140 | 20.561 | 38.192 | 31.883 | 1.00 | 47.96 | 7 |
| 10 | ATOM | 2743 | CA | ILE | B | 140 | 21.348 | 38.480 | 30.696 | 1.00 | 49.36 | 6 |
| | ATOM | 2744 | CB | ILE | B | 140 | 22.590 | 37.531 | 30.607 | 1.00 | 49.96 | 6 |
| | ATOM | 2745 | CG2 | ILE | B | 140 | 23.254 | 37.411 | 31.973 | 1.00 | 52.22 | 6 |
| | ATOM | 2746 | CG1 | ILE | B | 140 | 22.192 | 36.126 | 30.217 | 1.00 | 50.93 | 6 |
| | ATOM | 2747 | CD1 | ILE | B | 140 | 23.312 | 35.115 | 30.483 | 1.00 | 54.24 | 6 |
| | ATOM | 2748 | C | ILE | B | 140 | 20.520 | 38.444 | 29.410 | 1.00 | 48.36 | 6 |
| 15 | ATOM | 2749 | O | ILE | B | 140 | 19.727 | 37.545 | 29.211 | 1.00 | 49.73 | 8 |
| | ATOM | 2750 | N | GLY | B | 141 | 20.685 | 39.448 | 28.557 | 1.00 | 46.46 | 7 |
| | ATOM | 2751 | CA | GLY | B | 141 | 19.941 | 39.500 | 27.313 | 1.00 | 47.33 | 6 |
| | ATOM | 2752 | C | GLY | B | 141 | 20.631 | 40.387 | 26.293 | 1.00 | 46.71 | 6 |
| | ATOM | 2753 | O | GLY | B | 141 | 21.623 | 41.025 | 26.625 | 1.00 | 47.72 | 8 |
| 20 | ATOM | 2754 | N | SER | B | 142 | 20.131 | 40.425 | 25.058 | 1.00 | 45.43 | 7 |
| | ATOM | 2755 | CA | SER | B | 142 | 20.739 | 41.267 | 24.026 | 1.00 | 44.63 | 6 |
| | ATOM | 2756 | CB | SER | B | 142 | 19.990 | 41.165 | 22.706 | 1.00 | 42.45 | 6 |
| | ATOM | 2757 | OG | SER | B | 142 | 20.431 | 42.168 | 21.814 | 1.00 | 40.68 | 8 |
| | ATOM | 2758 | C | SER | B | 142 | 20.774 | 42.728 | 24.457 | 1.00 | 46.01 | 6 |
| 25 | ATOM | 2759 | O | SER | B | 142 | 19.812 | 43.256 | 25.031 | 1.00 | 46.34 | 8 |
| | ATOM | 2760 | N | TRP | B | 143 | 21.888 | 43.384 | 24.162 | 1.00 | 46.69 | 7 |
| | ATOM | 2761 | CA | TRP | B | 143 | 22.069 | 44.761 | 24.549 | 1.00 | 45.07 | 6 |
| | ATOM | 2762 | CB | TRP | B | 143 | 23.553 | 45.044 | 24.758 | 1.00 | 44.45 | 6 |
| | ATOM | 2763 | CG | TRP | B | 143 | 23.816 | 46.368 | 25.388 | 1.00 | 43.71 | 6 |
| 30 | ATOM | 2764 | CD2 | TRP | B | 143 | 23.642 | 46.697 | 26.762 | 1.00 | 40.44 | 6 |
| | ATOM | 2765 | CE2 | TRP | B | 143 | 23.999 | 48.055 | 26.920 | 1.00 | 40.05 | 6 |
| | ATOM | 2766 | CE3 | TRP | B | 143 | 23.221 | 45.975 | 27.880 | 1.00 | 38.96 | 6 |
| | ATOM | 2767 | CD1 | TRP | B | 143 | 24.262 | 47.517 | 24.773 | 1.00 | 43.74 | 6 |
| | ATOM | 2768 | NE1 | TRP | B | 143 | 24.373 | 48.534 | 25.691 | 1.00 | 40.21 | 7 |
| 35 | ATOM | 2769 | CZ2 | TRP | B | 143 | 23.947 | 48.694 | 28.149 | 1.00 | 38.81 | 6 |
| | ATOM | 2770 | CZ3 | TRP | B | 143 | 23.171 | 46.612 | 29.097 | 1.00 | 35.11 | 6 |
| | ATOM | 2771 | CH2 | TRP | B | 143 | 23.531 | 47.956 | 29.224 | 1.00 | 37.51 | 6 |
| | ATOM | 2772 | C | TRP | B | 143 | 21.499 | 45.730 | 23.545 | 1.00 | 46.35 | 6 |
| | ATOM | 2773 | O | TRP | B | 143 | 21.062 | 46.813 | 23.909 | 1.00 | 48.58 | 8 |
| 40 | ATOM | 2774 | N | THR | B | 144 | 21.477 | 45.358 | 22.277 | 1.00 | 45.22 | 7 |
| | ATOM | 2775 | CA | THR | B | 144 | 20.963 | 46.287 | 21.290 | 1.00 | 45.21 | 6 |
| | ATOM | 2776 | CB | THR | B | 144 | 22.072 | 46.696 | 20.328 | 1.00 | 44.02 | 6 |
| | ATOM | 2777 | OG1 | THR | B | 144 | 22.669 | 45.524 | 19.763 | 1.00 | 44.19 | 8 |
| | ATOM | 2778 | CG2 | THR | B | 144 | 23.129 | 47.487 | 21.069 | 1.00 | 42.50 | 6 |
| 45 | ATOM | 2779 | C | THR | B | 144 | 19.778 | 45.793 | 20.485 | 1.00 | 48.06 | 6 |
| | ATOM | 2780 | O | THR | B | 144 | 19.136 | 46.576 | 19.783 | 1.00 | 50.29 | 8 |
| | ATOM | 2781 | N | HIS | B | 145 | 19.474 | 44.504 | 20.584 | 1.00 | 47.78 | 7 |
| | ATOM | 2782 | CA | HIS | B | 145 | 18.364 | 43.970 | 19.820 | 1.00 | 48.99 | 6 |
| | ATOM | 2783 | CB | HIS | B | 145 | 18.800 | 42.716 | 19.055 | 1.00 | 47.81 | 6 |
| 50 | ATOM | 2784 | CG | HIS | B | 145 | 19.805 | 42.974 | 17.974 | 1.00 | 46.09 | 6 |
| | ATOM | 2785 | CD2 | HIS | B | 145 | 19.677 | 43.532 | 16.748 | 1.00 | 44.37 | 6 |
| | ATOM | 2786 | ND1 | HIS | B | 145 | 21.125 | 42.602 | 18.086 | 1.00 | 45.57 | 7 |
| | ATOM | 2787 | CE1 | HIS | B | 145 | 21.766 | 42.915 | 16.975 | 1.00 | 44.33 | 6 |
| | ATOM | 2788 | NE2 | HIS | B | 145 | 20.909 | 43.481 | 16.146 | 1.00 | 41.88 | 7 |
| 55 | ATOM | 2789 | C | HIS | B | 145 | 17.149 | 43.656 | 20.682 | 1.00 | 50.77 | 6 |
| | ATOM | 2790 | O | HIS | B | 145 | 17.235 | 42.933 | 21.668 | 1.00 | 52.14 | 8 |
| | ATOM | 2791 | N | HIS | B | 146 | 16.010 | 44.213 | 20.302 | 1.00 | 52.05 | 7 |
| | ATOM | 2792 | CA | HIS | B | 146 | 14.774 | 43.974 | 21.027 | 1.00 | 54.32 | 6 |
| | ATOM | 2793 | CB | HIS | B | 146 | 13.797 | 45.130 | 20.800 | 1.00 | 52.48 | 6 |
| 60 | ATOM | 2794 | CG | HIS | B | 146 | 13.526 | 45.413 | 19.360 | 1.00 | 52.25 | 6 |
| | ATOM | 2795 | CD2 | HIS | B | 146 | 13.106 | 44.605 | 18.357 | 1.00 | 53.49 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2796 | ND1 | HIS | B | 146 | 13.726 | 46.653 | 18.795 | 1.00 | 53.68 | 7 |
| | ATOM | 2797 | CE1 | HIS | B | 146 | 13.448 | 46.597 | 17.504 | 1.00 | 55.84 | 6 |
| | ATOM | 2798 | NE2 | HIS | B | 146 | 13.070 | 45.364 | 17.212 | 1.00 | 55.30 | 7 |
| | ATOM | 2799 | C | HIS | B | 146 | 14.149 | 42.647 | 20.576 | 1.00 | 57.05 | 6 |
| 5 | ATOM | 2800 | O | HIS | B | 146 | 14.640 | 41.984 | 19.644 | 1.00 | 58.04 | 8 |
| | ATOM | 2801 | N | SER | B | 147 | 13.057 | 42.280 | 21.243 | 1.00 | 58.47 | 7 |
| | ATOM | 2802 | CA | SER | B | 147 | 12.328 | 41.037 | 20.997 | 1.00 | 58.52 | 6 |
| | ATOM | 2803 | CB | SER | B | 147 | 11.071 | 41.021 | 21.861 | 1.00 | 58.93 | 6 |
| | ATOM | 2804 | OG | SER | B | 147 | 10.386 | 42.252 | 21.740 | 1.00 | 63.53 | 8 |
| 10 | ATOM | 2805 | C | SER | B | 147 | 11.955 | 40.708 | 19.557 | 1.00 | 57.13 | 6 |
| | ATOM | 2806 | O | SER | B | 147 | 11.776 | 39.545 | 19.215 | 1.00 | 56.86 | 8 |
| | ATOM | 2807 | N | ARG | B | 148 | 11.841 | 41.716 | 18.709 | 1.00 | 56.50 | 7 |
| | ATOM | 2808 | CA | ARG | B | 148 | 11.473 | 41.462 | 17.323 | 1.00 | 58.81 | 6 |
| | ATOM | 2809 | CB | ARG | B | 148 | 10.905 | 42.734 | 16.691 | 1.00 | 62.56 | 6 |
| 15 | ATOM | 2810 | CG | ARG | B | 148 | 9.781 | 43.380 | 17.493 | 1.00 | 70.38 | 6 |
| | ATOM | 2811 | CD | ARG | B | 148 | 9.337 | 44.731 | 16.897 | 1.00 | 76.49 | 6 |
| | ATOM | 2812 | NE | ARG | B | 148 | 8.480 | 45.487 | 17.819 | 1.00 | 82.57 | 7 |
| | ATOM | 2813 | CZ | ARG | B | 148 | 7.263 | 45.104 | 18.222 | 1.00 | 84.74 | 6 |
| | ATOM | 2814 | NH1 | ARG | B | 148 | 6.728 | 43.965 | 17.791 | 1.00 | 85.52 | 7 |
| 20 | ATOM | 2815 | NH2 | ARG | B | 148 | 6.573 | 45.864 | 19.064 | 1.00 | 85.55 | 7 |
| | ATOM | 2816 | C | ARG | B | 148 | 12.655 | 40.963 | 16.490 | 1.00 | 57.83 | 6 |
| | ATOM | 2817 | O | ARG | B | 148 | 12.474 | 40.423 | 15.395 | 1.00 | 58.23 | 8 |
| | ATOM | 2818 | N | GLU | B | 149 | 13.864 | 41.147 | 17.011 | 1.00 | 56.99 | 7 |
| | ATOM | 2819 | CA | GLU | B | 149 | 15.072 | 40.743 | 16.306 | 1.00 | 53.60 | 6 |
| 25 | ATOM | 2820 | CB | GLU | B | 149 | 16.015 | 41.933 | 16.216 | 1.00 | 52.91 | 6 |
| | ATOM | 2821 | CG | GLU | B | 149 | 15.280 | 43.243 | 15.955 | 1.00 | 51.82 | 6 |
| | ATOM | 2822 | CD | GLU | B | 149 | 16.208 | 44.437 | 15.841 | 1.00 | 54.76 | 6 |
| | ATOM | 2823 | OE1 | GLU | B | 149 | 17.132 | 44.562 | 16.672 | 1.00 | 55.52 | 8 |
| | ATOM | 2824 | OE2 | GLU | B | 149 | 16.010 | 45.261 | 14.929 | 1.00 | 52.75 | 8 |
| 30 | ATOM | 2825 | C | GLU | B | 149 | 15.729 | 39.584 | 17.036 | 1.00 | 52.38 | 6 |
| | ATOM | 2826 | O | GLU | B | 149 | 16.150 | 38.606 | 16.421 | 1.00 | 51.81 | 8 |
| | ATOM | 2827 | N | ILE | B | 150 | 15.811 | 39.693 | 18.355 | 1.00 | 51.32 | 7 |
| | ATOM | 2828 | CA | ILE | B | 150 | 16.382 | 38.619 | 19.154 | 1.00 | 51.11 | 6 |
| | ATOM | 2829 | CB | ILE | B | 150 | 17.770 | 38.989 | 19.757 | 1.00 | 48.77 | 6 |
| 35 | ATOM | 2830 | CG2 | ILE | B | 150 | 18.155 | 37.995 | 20.843 | 1.00 | 43.40 | 6 |
| | ATOM | 2831 | CG1 | ILE | B | 150 | 18.842 | 38.967 | 18.672 | 1.00 | 47.30 | 6 |
| | ATOM | 2832 | CD1 | ILE | B | 150 | 20.219 | 39.315 | 19.168 | 1.00 | 45.12 | 6 |
| | ATOM | 2833 | C | ILE | B | 150 | 15.453 | 38.254 | 20.297 | 1.00 | 53.02 | 6 |
| | ATOM | 2834 | O | ILE | B | 150 | 14.842 | 39.116 | 20.932 | 1.00 | 52.00 | 8 |
| 40 | ATOM | 2835 | N | SER | B | 151 | 15.350 | 36.955 | 20.539 | 1.00 | 55.16 | 7 |
| | ATOM | 2836 | CA | SER | B | 151 | 14.542 | 36.436 | 21.628 | 1.00 | 56.52 | 6 |
| | ATOM | 2837 | CB | SER | B | 151 | 13.280 | 35.733 | 21.089 | 1.00 | 57.06 | 6 |
| | ATOM | 2838 | OG | SER | B | 151 | 13.594 | 34.585 | 20.323 | 1.00 | 54.91 | 8 |
| | ATOM | 2839 | C | SER | B | 151 | 15.452 | 35.447 | 22.337 | 1.00 | 56.69 | 6 |
| 45 | ATOM | 2840 | O | SER | B | 151 | 16.144 | 34.676 | 21.685 | 1.00 | 57.55 | 8 |
| | ATOM | 2841 | N | VAL | B | 152 | 15.480 | 35.504 | 23.661 | 1.00 | 58.35 | 7 |
| | ATOM | 2842 | CA | VAL | B | 152 | 16.306 | 34.600 | 24.456 | 1.00 | 60.89 | 6 |
| | ATOM | 2843 | CB | VAL | B | 152 | 17.135 | 35.362 | 25.502 | 1.00 | 60.77 | 6 |
| | ATOM | 2844 | CG1 | VAL | B | 152 | 17.890 | 36.489 | 24.844 | 1.00 | 59.09 | 6 |
| 50 | ATOM | 2845 | CG2 | VAL | B | 152 | 16.220 | 35.903 | 26.586 | 1.00 | 62.75 | 6 |
| | ATOM | 2846 | C | VAL | B | 152 | 15.389 | 33.632 | 25.194 | 1.00 | 62.80 | 6 |
| | ATOM | 2847 | O | VAL | B | 152 | 14.287 | 34.012 | 25.597 | 1.00 | 63.08 | 8 |
| | ATOM | 2848 | N | ASP | B | 153 | 15.845 | 32.395 | 25.387 | 1.00 | 64.20 | 7 |
| | ATOM | 2849 | CA | ASP | B | 153 | 15.028 | 31.390 | 26.061 | 1.00 | 66.36 | 6 |
| 55 | ATOM | 2850 | CB | ASP | B | 153 | 14.232 | 30.611 | 25.016 | 1.00 | 67.03 | 6 |
| | ATOM | 2851 | CG | ASP | B | 153 | 13.427 | 31.518 | 24.095 | 1.00 | 68.33 | 6 |
| | ATOM | 2852 | OD1 | ASP | B | 153 | 12.327 | 31.949 | 24.504 | 1.00 | 65.39 | 8 |
| | ATOM | 2853 | OD2 | ASP | B | 153 | 13.905 | 31.810 | 22.969 | 1.00 | 70.09 | 8 |
| | ATOM | 2854 | C | ASP | B | 153 | 15.877 | 30.416 | 26.872 | 1.00 | 68.77 | 6 |
| 60 | ATOM | 2855 | O | ASP | B | 153 | 16.974 | 30.049 | 26.453 | 1.00 | 69.28 | 8 |
| | ATOM | 2856 | N | PRO | B | 154 | 15.404 | 30.017 | 28.067 | 1.00 | 70.46 | 7 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|---|
| | ATOM | 2857 | CD | PRO | B | 154 | 14.409 | 30.740 | 28.876 | 1.00 | 69.92 | 6 |
| | ATOM | 2858 | CA | PRO | B | 154 | 16.157 | 29.070 | 28.898 | 1.00 | 72.29 | 6 |
| | ATOM | 2859 | CB | PRO | B | 154 | 15.410 | 29.108 | 30.225 | 1.00 | 70.76 | 6 |
| | ATOM | 2860 | CG | PRO | B | 154 | 14.902 | 30.494 | 30.281 | 1.00 | 69.28 | 6 |
| 5 | ATOM | 2861 | C | PRO | B | 154 | 16.151 | 27.668 | 28.250 | 1.00 | 75.71 | 6 |
| | ATOM | 2862 | O | PRO | B | 154 | 15.548 | 27.467 | 27.187 | 1.00 | 75.41 | 8 |
| | ATOM | 2863 | N | THR | B | 155 | 16.807 | 26.700 | 28.888 | 1.00 | 79.33 | 7 |
| | ATOM | 2864 | CA | THR | B | 155 | 16.887 | 25.350 | 28.332 | 1.00 | 83.13 | 6 |
| | ATOM | 2865 | CB | THR | B | 155 | 18.208 | 25.187 | 27.542 | 1.00 | 82.37 | 6 |
| 10 | ATOM | 2866 | OG1 | THR | B | 155 | 19.316 | 25.233 | 28.453 | 1.00 | 83.94 | 8 |
| | ATOM | 2867 | CG2 | THR | B | 155 | 18.378 | 26.311 | 26.545 | 1.00 | 81.49 | 6 |
| | ATOM | 2868 | C | THR | B | 155 | 16.785 | 24.189 | 29.348 | 1.00 | 86.65 | 6 |
| | ATOM | 2869 | O | THR | B | 155 | 16.122 | 24.298 | 30.385 | 1.00 | 87.45 | 8 |
| | ATOM | 2870 | N | THR | B | 156 | 17.452 | 23.078 | 29.013 | 1.00 | 90.57 | 7 |
| 15 | ATOM | 2871 | CA | THR | B | 156 | 17.504 | 21.839 | 29.813 | 1.00 | 93.48 | 6 |
| | ATOM | 2872 | CB | THR | B | 156 | 18.799 | 21.025 | 29.491 | 1.00 | 93.70 | 6 |
| | ATOM | 2873 | OG1 | THR | B | 156 | 18.861 | 20.761 | 28.077 | 1.00 | 92.52 | 8 |
| | ATOM | 2874 | CG2 | THR | B | 156 | 18.825 | 19.694 | 30.301 | 1.00 | 93.12 | 6 |
| | ATOM | 2875 | C | THR | B | 156 | 17.448 | 22.012 | 31.337 | 1.00 | 95.82 | 6 |
| 20 | ATOM | 2876 | O | THR | B | 156 | 18.471 | 22.286 | 31.990 | 1.00 | 95.51 | 8 |
| | ATOM | 2877 | N | GLU | B | 157 | 16.257 | 21.809 | 31.897 | 1.00 | 98.15 | 7 |
| | ATOM | 2878 | CA | GLU | B | 157 | 16.047 | 21.946 | 33.337 | 1.00 | 100.26 | 6 |
| | ATOM | 2879 | CB | GLU | B | 157 | 14.583 | 22.308 | 33.606 | 1.00 | 102.01 | 6 |
| | ATOM | 2880 | CG | GLU | B | 157 | 14.023 | 23.363 | 32.643 | 1.00 | 104.88 | 6 |
| 25 | ATOM | 2881 | CD | GLU | B | 157 | 12.539 | 23.649 | 32.902 | 1.00 | 106.35 | 6 |
| | ATOM | 2882 | OE1 | GLU | B | 157 | 11.745 | 22.665 | 32.965 | 1.00 | 106.79 | 8 |
| | ATOM | 2883 | OE2 | GLU | B | 157 | 12.178 | 24.850 | 33.030 | 1.00 | 105.97 | 8 |
| | ATOM | 2884 | C | GLU | B | 157 | 16.397 | 20.662 | 34.102 | 1.00 | 100.31 | 6 |
| | ATOM | 2885 | O | GLU | B | 157 | 16.352 | 20.631 | 35.348 | 1.00 | 100.47 | 8 |
| 30 | ATOM | 2886 | N | ASN | B | 158 | 16.726 | 19.601 | 33.364 | 1.00 | 99.66 | 7 |
| | ATOM | 2887 | CA | ASN | B | 158 | 17.065 | 18.329 | 34.003 | 1.00 | 99.04 | 6 |
| | ATOM | 2888 | CB | ASN | B | 158 | 17.084 | 17.198 | 32.969 | 1.00 | 100.65 | 6 |
| | ATOM | 2889 | CG | ASN | B | 158 | 15.793 | 17.113 | 32.170 | 1.00 | 101.63 | 6 |
| | ATOM | 2890 | OD1 | ASN | B | 158 | 14.701 | 16.919 | 32.733 | 1.00 | 101.77 | 8 |
| 35 | ATOM | 2891 | ND2 | ASN | B | 158 | 15.909 | 17.254 | 30.847 | 1.00 | 102.28 | 7 |
| | ATOM | 2892 | C | ASN | B | 158 | 18.439 | 18.424 | 34.672 | 1.00 | 97.31 | 6 |
| | ATOM | 2893 | O | ASN | B | 158 | 18.546 | 18.748 | 35.872 | 1.00 | 97.45 | 8 |
| | ATOM | 2894 | N | SER | B | 159 | 19.473 | 18.120 | 33.881 | 1.00 | 94.36 | 7 |
| | ATOM | 2895 | CA | SER | B | 159 | 20.879 | 18.156 | 34.300 | 1.00 | 90.64 | 6 |
| 40 | ATOM | 2896 | CB | SER | B | 159 | 21.645 | 19.051 | 33.325 | 1.00 | 91.05 | 6 |
| | ATOM | 2897 | OG | SER | B | 159 | 20.831 | 20.167 | 32.948 | 1.00 | 91.42 | 8 |
| | ATOM | 2898 | C | SER | B | 159 | 21.129 | 18.622 | 35.742 | 1.00 | 87.58 | 6 |
| | ATOM | 2899 | O | SER | B | 159 | 20.770 | 19.741 | 36.114 | 1.00 | 87.04 | 8 |
| | ATOM | 2900 | N | ASP | B | 160 | 21.744 | 17.767 | 36.553 | 1.00 | 84.29 | 7 |
| 45 | ATOM | 2901 | CA | ASP | B | 160 | 22.035 | 18.137 | 37.938 | 1.00 | 80.73 | 6 |
| | ATOM | 2902 | CB | ASP | B | 160 | 23.003 | 17.149 | 38.582 | 1.00 | 79.96 | 6 |
| | ATOM | 2903 | CG | ASP | B | 160 | 23.404 | 17.566 | 39.991 | 1.00 | 79.90 | 6 |
| | ATOM | 2904 | OD1 | ASP | B | 160 | 24.459 | 17.087 | 40.471 | 1.00 | 79.39 | 8 |
| | ATOM | 2905 | OD2 | ASP | B | 160 | 22.659 | 18.362 | 40.617 | 1.00 | 79.13 | 8 |
| 50 | ATOM | 2906 | C | ASP | B | 160 | 22.687 | 19.514 | 37.956 | 1.00 | 79.03 | 6 |
| | ATOM | 2907 | O | ASP | B | 160 | 23.782 | 19.687 | 37.394 | 1.00 | 78.08 | 8 |
| | ATOM | 2908 | N | ASP | B | 161 | 22.022 | 20.473 | 38.612 | 1.00 | 76.06 | 7 |
| | ATOM | 2909 | CA | ASP | B | 161 | 22.506 | 21.851 | 38.706 | 1.00 | 71.50 | 6 |
| | ATOM | 2910 | CB | ASP | B | 161 | 21.655 | 22.683 | 39.675 | 1.00 | 70.10 | 6 |
| 55 | ATOM | 2911 | CG | ASP | B | 161 | 20.275 | 22.977 | 39.130 | 1.00 | 69.41 | 6 |
| | ATOM | 2912 | OD1 | ASP | B | 161 | 20.140 | 23.189 | 37.905 | 1.00 | 68.26 | 8 |
| | ATOM | 2913 | OD2 | ASP | B | 161 | 19.319 | 23.007 | 39.929 | 1.00 | 71.44 | 8 |
| | ATOM | 2914 | C | ASP | B | 161 | 23.957 | 21.979 | 39.110 | 1.00 | 69.84 | 6 |
| | ATOM | 2915 | O | ASP | B | 161 | 24.569 | 23.008 | 38.843 | 1.00 | 71.09 | 8 |
| 60 | ATOM | 2916 | N | SER | B | 162 | 24.527 | 20.960 | 39.740 | 1.00 | 67.23 | 7 |
| | ATOM | 2917 | CA | SER | B | 162 | 25.928 | 21.078 | 40.136 | 1.00 | 67.27 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|---------|
| 5 | ATOM | 2918 | CB | SER B 162 | 26.051 | 21.210 | 41.661 | 1.00 | 67.18 6 |
| | ATOM | 2919 | OG | SER B 162 | 25.648 | 20.020 | 42.315 | 1.00 | 66.16 8 |
| | ATOM | 2920 | C | SER B 162 | 26.787 | 19.922 | 39.653 | 1.00 | 66.71 6 |
| | ATOM | 2921 | O | SER B 162 | 27.786 | 19.576 | 40.289 | 1.00 | 64.25 8 |
| | ATOM | 2922 | N | GLU B 163 | 26.410 | 19.330 | 38.523 | 1.00 | 67.10 7 |
| 10 | ATOM | 2923 | CA | GLU B 163 | 27.192 | 18.220 | 38.005 | 1.00 | 68.36 6 |
| | ATOM | 2924 | CB | GLU B 163 | 26.378 | 17.421 | 36.970 | 1.00 | 70.98 6 |
| | ATOM | 2925 | CG | GLU B 163 | 26.411 | 17.926 | 35.545 | 1.00 | 72.60 6 |
| | ATOM | 2926 | CD | GLU B 163 | 25.726 | 16.946 | 34.594 | 1.00 | 74.62 6 |
| | ATOM | 2927 | OE1 | GLU B 163 | 24.477 | 16.828 | 34.649 | 1.00 | 76.45 8 |
| 15 | ATOM | 2928 | OE2 | GLU B 163 | 26.428 | 16.285 | 33.798 | 1.00 | 74.37 8 |
| | ATOM | 2929 | C | GLU B 163 | 28.530 | 18.688 | 37.410 | 1.00 | 67.51 6 |
| | ATOM | 2930 | O | GLU B 163 | 29.379 | 17.868 | 37.070 | 1.00 | 67.13 8 |
| | ATOM | 2931 | N | TYR B 164 | 28.709 | 20.008 | 37.294 | 1.00 | 66.57 7 |
| | ATOM | 2932 | CA | TYR B 164 | 29.943 | 20.583 | 36.771 | 1.00 | 64.39 6 |
| 20 | ATOM | 2933 | CB | TYR B 164 | 29.671 | 21.419 | 35.526 | 1.00 | 64.28 6 |
| | ATOM | 2934 | CG | TYR B 164 | 29.192 | 20.602 | 34.354 | 1.00 | 66.44 6 |
| | ATOM | 2935 | CD1 | TYR B 164 | 27.948 | 20.860 | 33.766 | 1.00 | 66.70 6 |
| | ATOM | 2936 | CE1 | TYR B 164 | 27.490 | 20.105 | 32.690 | 1.00 | 66.59 6 |
| | ATOM | 2937 | CD2 | TYR B 164 | 29.973 | 19.556 | 33.832 | 1.00 | 65.02 6 |
| 25 | ATOM | 2938 | CE2 | TYR B 164 | 29.524 | 18.790 | 32.756 | 1.00 | 65.71 6 |
| | ATOM | 2939 | CZ | TYR B 164 | 28.277 | 19.075 | 32.184 | 1.00 | 66.77 6 |
| | ATOM | 2940 | OH | TYR B 164 | 27.819 | 18.369 | 31.084 | 1.00 | 67.83 8 |
| | ATOM | 2941 | C | TYR B 164 | 30.584 | 21.463 | 37.826 | 1.00 | 63.28 6 |
| | ATOM | 2942 | O | TYR B 164 | 31.717 | 21.936 | 37.662 | 1.00 | 61.67 8 |
| 30 | ATOM | 2943 | N | PHE B 165 | 29.859 | 21.673 | 38.918 | 1.00 | 61.88 7 |
| | ATOM | 2944 | CA | PHE B 165 | 30.357 | 22.517 | 39.990 | 1.00 | 60.70 6 |
| | ATOM | 2945 | CB | PHE B 165 | 29.288 | 22.704 | 41.067 | 1.00 | 58.78 6 |
| | ATOM | 2946 | CG | PHE B 165 | 29.523 | 23.905 | 41.941 | 1.00 | 57.08 6 |
| | ATOM | 2947 | CD1 | PHE B 165 | 29.420 | 25.184 | 41.413 | 1.00 | 56.05 6 |
| 35 | ATOM | 2948 | CD2 | PHE B 165 | 29.888 | 23.757 | 43.272 | 1.00 | 54.09 6 |
| | ATOM | 2949 | CE1 | PHE B 165 | 29.680 | 26.296 | 42.200 | 1.00 | 55.95 6 |
| | ATOM | 2950 | CE2 | PHE B 165 | 30.149 | 24.858 | 44.063 | 1.00 | 55.48 6 |
| | ATOM | 2951 | CZ | PHE B 165 | 30.048 | 26.131 | 43.530 | 1.00 | 56.15 6 |
| | ATOM | 2952 | C | PHE B 165 | 31.626 | 21.960 | 40.614 | 1.00 | 59.91 6 |
| 40 | ATOM | 2953 | O | PHE B 165 | 31.757 | 20.760 | 40.808 | 1.00 | 60.17 8 |
| | ATOM | 2954 | N | SER B 166 | 32.572 | 22.839 | 40.919 | 1.00 | 60.28 7 |
| | ATOM | 2955 | CA | SER B 166 | 33.807 | 22.390 | 41.532 | 1.00 | 60.24 6 |
| | ATOM | 2956 | CB | SER B 166 | 34.810 | 23.534 | 41.647 | 1.00 | 59.33 6 |
| | ATOM | 2957 | OG | SER B 166 | 36.012 | 23.081 | 42.239 | 1.00 | 59.12 8 |
| 45 | ATOM | 2958 | C | SER B 166 | 33.468 | 21.877 | 42.916 | 1.00 | 60.82 6 |
| | ATOM | 2959 | O | SER B 166 | 32.614 | 22.434 | 43.611 | 1.00 | 60.12 8 |
| | ATOM | 2960 | N | GLN B 167 | 34.148 | 20.815 | 43.319 | 1.00 | 61.73 7 |
| | ATOM | 2961 | CA | GLN B 167 | 33.907 | 20.228 | 44.623 | 1.00 | 62.29 6 |
| | ATOM | 2962 | CB | GLN B 167 | 34.228 | 18.737 | 44.576 | 1.00 | 63.96 6 |
| 50 | ATOM | 2963 | CG | GLN B 167 | 35.620 | 18.442 | 44.068 | 1.00 | 66.77 6 |
| | ATOM | 2964 | CD | GLN B 167 | 35.827 | 16.969 | 43.736 | 1.00 | 68.16 6 |
| | ATOM | 2965 | OE1 | GLN B 167 | 35.710 | 16.103 | 44.605 | 1.00 | 66.24 8 |
| | ATOM | 2966 | NE2 | GLN B 167 | 36.136 | 16.682 | 42.465 | 1.00 | 68.10 7 |
| | ATOM | 2967 | C | GLN B 167 | 34.740 | 20.912 | 45.689 | 1.00 | 60.72 6 |
| 55 | ATOM | 2968 | O | GLN B 167 | 34.433 | 20.814 | 46.880 | 1.00 | 62.24 8 |
| | ATOM | 2969 | N | TYR B 168 | 35.778 | 21.626 | 45.269 | 1.00 | 57.81 7 |
| | ATOM | 2970 | CA | TYR B 168 | 36.637 | 22.291 | 46.235 | 1.00 | 56.47 6 |
| | ATOM | 2971 | CB | TYR B 168 | 38.078 | 22.236 | 45.741 | 1.00 | 55.55 6 |
| | ATOM | 2972 | CG | TYR B 168 | 38.457 | 20.836 | 45.330 | 1.00 | 55.77 6 |
| 60 | ATOM | 2973 | CD1 | TYR B 168 | 38.420 | 20.447 | 43.988 | 1.00 | 53.38 6 |
| | ATOM | 2974 | CE1 | TYR B 168 | 38.698 | 19.139 | 43.617 | 1.00 | 53.39 6 |
| | ATOM | 2975 | CD2 | TYR B 168 | 38.785 | 19.872 | 46.286 | 1.00 | 55.32 6 |
| | ATOM | 2976 | CE2 | TYR B 168 | 39.060 | 18.561 | 45.922 | 1.00 | 54.41 6 |
| | ATOM | 2977 | CZ | TYR B 168 | 39.013 | 18.207 | 44.591 | 1.00 | 54.89 6 |
| | ATOM | 2978 | OH | TYR B 168 | 39.270 | 16.919 | 44.227 | 1.00 | 56.81 8 |

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|----|------|------|-----|-----------|--------|--------|--------|------|---------|
| 5 | ATOM | 2979 | C | TYR B 168 | 36.222 | 23.712 | 46.586 | 1.00 | 55.31 6 |
| | ATOM | 2980 | O | TYR B 168 | 36.891 | 24.395 | 47.356 | 1.00 | 54.88 8 |
| | ATOM | 2981 | N | SER B 169 | 35.097 | 24.140 | 46.033 | 1.00 | 55.16 7 |
| | ATOM | 2982 | CA | SER B 169 | 34.570 | 25.469 | 46.299 | 1.00 | 57.04 6 |
| | ATOM | 2983 | CB | SER B 169 | 33.363 | 25.755 | 45.412 | 1.00 | 55.22 6 |
| 10 | ATOM | 2984 | OG | SER B 169 | 32.775 | 26.991 | 45.769 | 1.00 | 55.21 8 |
| | ATOM | 2985 | C | SER B 169 | 34.147 | 25.617 | 47.754 | 1.00 | 60.21 6 |
| | ATOM | 2986 | O | SER B 169 | 33.664 | 24.671 | 48.380 | 1.00 | 62.02 8 |
| | ATOM | 2987 | N | ARG B 170 | 34.321 | 26.815 | 48.298 | 1.00 | 61.79 7 |
| | ATOM | 2988 | CA | ARG B 170 | 33.938 | 27.059 | 49.678 | 1.00 | 60.59 6 |
| 15 | ATOM | 2989 | CB | ARG B 170 | 34.467 | 28.417 | 50.150 | 1.00 | 61.26 6 |
| | ATOM | 2990 | CG | ARG B 170 | 35.781 | 28.342 | 50.904 | 1.00 | 61.61 6 |
| | ATOM | 2991 | CD | ARG B 170 | 36.588 | 29.628 | 50.764 | 1.00 | 66.75 6 |
| | ATOM | 2992 | NE | ARG B 170 | 35.866 | 30.846 | 51.158 | 1.00 | 69.32 7 |
| | ATOM | 2993 | CZ | ARG B 170 | 35.634 | 31.877 | 50.342 | 1.00 | 68.59 6 |
| 20 | ATOM | 2994 | NH1 | ARG B 170 | 36.053 | 31.840 | 49.079 | 1.00 | 65.59 7 |
| | ATOM | 2995 | NH2 | ARG B 170 | 35.017 | 32.959 | 50.803 | 1.00 | 69.04 7 |
| | ATOM | 2996 | C | ARG B 170 | 32.431 | 27.041 | 49.785 | 1.00 | 58.91 6 |
| | ATOM | 2997 | O | ARG B 170 | 31.892 | 26.981 | 50.883 | 1.00 | 61.10 8 |
| | ATOM | 2998 | N | PHE B 171 | 31.748 | 27.077 | 48.650 | 1.00 | 56.02 7 |
| 25 | ATOM | 2999 | CA | PHE B 171 | 30.294 | 27.093 | 48.674 | 1.00 | 56.85 6 |
| | ATOM | 3000 | CB | PHE B 171 | 29.782 | 28.384 | 48.033 | 1.00 | 56.79 6 |
| | ATOM | 3001 | CG | PHE B 171 | 30.498 | 29.608 | 48.529 | 1.00 | 59.30 6 |
| | ATOM | 3002 | CD1 | PHE B 171 | 31.806 | 29.889 | 48.110 | 1.00 | 59.59 6 |
| | ATOM | 3003 | CD2 | PHE B 171 | 29.900 | 30.447 | 49.462 | 1.00 | 58.28 6 |
| 30 | ATOM | 3004 | CE1 | PHE B 171 | 32.497 | 30.983 | 48.616 | 1.00 | 58.87 6 |
| | ATOM | 3005 | CE2 | PHE B 171 | 30.586 | 31.546 | 49.978 | 1.00 | 57.19 6 |
| | ATOM | 3006 | CZ | PHE B 171 | 31.883 | 31.817 | 49.556 | 1.00 | 58.74 6 |
| | ATOM | 3007 | C | PHE B 171 | 29.694 | 25.892 | 47.987 | 1.00 | 57.50 6 |
| | ATOM | 3008 | O | PHE B 171 | 30.412 | 25.063 | 47.439 | 1.00 | 57.83 8 |
| 35 | ATOM | 3009 | N | GLU B 172 | 28.372 | 25.793 | 48.036 | 1.00 | 58.25 7 |
| | ATOM | 3010 | CA | GLU B 172 | 27.671 | 24.681 | 47.416 | 1.00 | 58.95 6 |
| | ATOM | 3011 | CB | GLU B 172 | 27.418 | 23.555 | 48.436 | 1.00 | 61.94 6 |
| | ATOM | 3012 | CG | GLU B 172 | 26.521 | 23.921 | 49.634 | 1.00 | 65.83 6 |
| | ATOM | 3013 | CD | GLU B 172 | 26.352 | 22.769 | 50.637 | 1.00 | 67.36 6 |
| 40 | ATOM | 3014 | OE1 | GLU B 172 | 26.275 | 21.593 | 50.192 | 1.00 | 67.12 8 |
| | ATOM | 3015 | OE2 | GLU B 172 | 26.280 | 23.043 | 51.868 | 1.00 | 67.97 8 |
| | ATOM | 3016 | C | GLU B 172 | 26.369 | 25.197 | 46.844 | 1.00 | 59.12 6 |
| | ATOM | 3017 | O | GLU B 172 | 25.837 | 26.217 | 47.302 | 1.00 | 58.48 8 |
| | ATOM | 3018 | N | ILE B 173 | 25.865 | 24.502 | 45.831 | 1.00 | 59.47 7 |
| 45 | ATOM | 3019 | CA | ILE B 173 | 24.630 | 24.911 | 45.180 | 1.00 | 60.85 6 |
| | ATOM | 3020 | CB | ILE B 173 | 24.715 | 24.729 | 43.653 | 1.00 | 62.04 6 |
| | ATOM | 3021 | CG2 | ILE B 173 | 23.369 | 25.077 | 42.998 | 1.00 | 60.25 6 |
| | ATOM | 3022 | CG1 | ILE B 173 | 25.832 | 25.603 | 43.087 | 1.00 | 62.02 6 |
| | ATOM | 3023 | CD1 | ILE B 173 | 26.018 | 25.413 | 41.600 | 1.00 | 63.88 6 |
| 50 | ATOM | 3024 | C | ILE B 173 | 23.415 | 24.148 | 45.667 | 1.00 | 61.72 6 |
| | ATOM | 3025 | O | ILE B 173 | 23.415 | 22.919 | 45.733 | 1.00 | 61.55 8 |
| | ATOM | 3026 | N | LEU B 174 | 22.369 | 24.883 | 45.999 | 1.00 | 62.91 7 |
| | ATOM | 3027 | CA | LEU B 174 | 21.158 | 24.253 | 46.460 | 1.00 | 63.63 6 |
| | ATOM | 3028 | CB | LEU B 174 | 20.438 | 25.166 | 47.443 | 1.00 | 63.66 6 |
| 55 | ATOM | 3029 | CG | LEU B 174 | 21.339 | 25.698 | 48.556 | 1.00 | 64.21 6 |
| | ATOM | 3030 | CD1 | LEU B 174 | 20.543 | 26.678 | 49.428 | 1.00 | 63.13 6 |
| | ATOM | 3031 | CD2 | LEU B 174 | 21.914 | 24.532 | 49.369 | 1.00 | 61.09 6 |
| | ATOM | 3032 | C | LEU B 174 | 20.307 | 24.010 | 45.232 | 1.00 | 64.20 6 |
| | ATOM | 3033 | O | LEU B 174 | 19.891 | 22.885 | 44.962 | 1.00 | 65.99 8 |
| 60 | ATOM | 3034 | N | ASP B 175 | 20.068 | 25.058 | 44.459 | 1.00 | 64.89 7 |
| | ATOM | 3035 | CA | ASP B 175 | 19.250 | 24.895 | 43.268 | 1.00 | 66.77 6 |
| | ATOM | 3036 | CB | ASP B 175 | 17.764 | 24.785 | 43.691 | 1.00 | 68.40 6 |
| | ATOM | 3037 | CG | ASP B 175 | 16.806 | 24.566 | 42.508 | 1.00 | 70.08 6 |
| | ATOM | 3038 | OD1 | ASP B 175 | 17.038 | 23.631 | 41.695 | 1.00 | 71.56 8 |
| | ATOM | 3039 | OD2 | ASP B 175 | 15.809 | 25.322 | 42.404 | 1.00 | 67.36 8 |

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|------|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3040 | C | ASP | B | 175 | 19.480 | 26.067 | 42.298 | 1.00 | 67.13 | 6 |
| | ATOM | 3041 | O | ASP | B | 175 | 19.910 | 27.160 | 42.703 | 1.00 | 67.04 | 8 |
| | ATOM | 3042 | N | VAL | B | 176 | 19.214 | 25.818 | 41.018 | 1.00 | 66.07 | 7 |
| | ATOM | 3043 | CA | VAL | B | 176 | 19.364 | 26.819 | 39.981 | 1.00 | 65.28 | 6 |
| | ATOM | 3044 | CB | VAL | B | 176 | 20.616 | 26.547 | 39.112 | 1.00 | 64.59 | 6 |
| | ATOM | 3045 | CG1 | VAL | B | 176 | 20.681 | 27.529 | 37.943 | 1.00 | 62.08 | 6 |
| | ATOM | 3046 | CG2 | VAL | B | 176 | 21.866 | 26.645 | 39.964 | 1.00 | 64.50 | 6 |
| 10 | ATOM | 3047 | C | VAL | B | 176 | 18.139 | 26.760 | 39.088 | 1.00 | 66.92 | 6 |
| | ATOM | 3048 | O | VAL | B | 176 | 17.723 | 25.682 | 38.657 | 1.00 | 68.14 | 8 |
| | ATOM | 3049 | N | THR | B | 177 | 17.555 | 27.920 | 38.816 | 1.00 | 68.01 | 7 |
| | ATOM | 3050 | CA | THR | B | 177 | 16.393 | 27.988 | 37.939 | 1.00 | 70.52 | 6 |
| | ATOM | 3051 | CB | THR | B | 177 | 15.087 | 28.139 | 38.744 | 1.00 | 69.59 | 6 |
| | ATOM | 3052 | OG1 | THR | B | 177 | 15.203 | 29.253 | 39.638 | 1.00 | 70.12 | 8 |
| | ATOM | 3053 | CG2 | THR | B | 177 | 14.821 | 26.885 | 39.544 | 1.00 | 68.35 | 6 |
| 15 | ATOM | 3054 | C | THR | B | 177 | 16.537 | 29.173 | 36.984 | 1.00 | 72.66 | 6 |
| | ATOM | 3055 | O | THR | B | 177 | 17.095 | 30.220 | 37.356 | 1.00 | 74.08 | 8 |
| | ATOM | 3056 | N | GLN | B | 178 | 16.049 | 29.002 | 35.757 | 1.00 | 73.01 | 7 |
| | ATOM | 3057 | CA | GLN | B | 178 | 16.121 | 30.057 | 34.756 | 1.00 | 74.26 | 6 |
| | ATOM | 3058 | CB | GLN | B | 178 | 17.006 | 29.619 | 33.594 | 1.00 | 76.29 | 6 |
| | ATOM | 3059 | CG | GLN | B | 178 | 18.090 | 28.628 | 33.984 | 1.00 | 79.92 | 6 |
| | ATOM | 3060 | CD | GLN | B | 178 | 19.227 | 28.575 | 32.959 | 1.00 | 83.13 | 6 |
| 20 | ATOM | 3061 | OE1 | GLN | B | 178 | 18.993 | 28.495 | 31.731 | 1.00 | 83.91 | 8 |
| | ATOM | 3062 | NE2 | GLN | B | 178 | 20.469 | 28.616 | 33.458 | 1.00 | 82.82 | 7 |
| | ATOM | 3063 | C | GLN | B | 178 | 14.725 | 30.354 | 34.232 | 1.00 | 73.95 | 6 |
| | ATOM | 3064 | O | GLN | B | 178 | 14.041 | 29.454 | 33.752 | 1.00 | 75.30 | 8 |
| | ATOM | 3065 | N | LYS | B | 179 | 14.306 | 31.611 | 34.310 | 1.00 | 73.25 | 7 |
| | ATOM | 3066 | CA | LYS | B | 179 | 12.978 | 31.995 | 33.837 | 1.00 | 72.86 | 6 |
| | ATOM | 3067 | CB | LYS | B | 179 | 12.076 | 32.307 | 35.030 | 1.00 | 75.19 | 6 |
| 25 | ATOM | 3068 | CG | LYS | B | 179 | 12.196 | 31.282 | 36.160 | 1.00 | 78.55 | 6 |
| | ATOM | 3069 | CD | LYS | B | 179 | 11.456 | 31.735 | 37.428 | 1.00 | 80.12 | 6 |
| | ATOM | 3070 | CE | LYS | B | 179 | 11.845 | 30.874 | 38.631 | 1.00 | 80.51 | 6 |
| | ATOM | 3071 | NZ | LYS | B | 179 | 13.320 | 30.987 | 38.927 | 1.00 | 81.19 | 7 |
| | ATOM | 3072 | C | LYS | B | 179 | 13.101 | 33.232 | 32.961 | 1.00 | 70.68 | 6 |
| | ATOM | 3073 | O | LYS | B | 179 | 13.411 | 34.311 | 33.455 | 1.00 | 70.88 | 8 |
| | ATOM | 3074 | N | LYS | B | 180 | 12.852 | 33.090 | 31.665 | 1.00 | 68.28 | 7 |
| 30 | ATOM | 3075 | CA | LYS | B | 180 | 12.970 | 34.242 | 30.776 | 1.00 | 68.69 | 6 |
| | ATOM | 3076 | CB | LYS | B | 180 | 12.873 | 33.792 | 29.305 | 1.00 | 66.36 | 6 |
| | ATOM | 3077 | CG | LYS | B | 180 | 11.517 | 33.383 | 28.831 | 1.00 | 61.57 | 6 |
| | ATOM | 3078 | CD | LYS | B | 180 | 10.763 | 34.578 | 28.296 | 1.00 | 62.84 | 6 |
| | ATOM | 3079 | CE | LYS | B | 180 | 11.419 | 35.168 | 27.058 | 1.00 | 63.27 | 6 |
| | ATOM | 3080 | NZ | LYS | B | 180 | 11.317 | 34.295 | 25.857 | 1.00 | 64.69 | 7 |
| | ATOM | 3081 | C | LYS | B | 180 | 11.914 | 35.297 | 31.096 | 1.00 | 69.36 | 6 |
| 35 | ATOM | 3082 | O | LYS | B | 180 | 11.131 | 35.112 | 32.019 | 1.00 | 70.64 | 8 |
| | ATOM | 3083 | N | ASN | B | 181 | 11.922 | 36.416 | 30.366 | 1.00 | 69.86 | 7 |
| | ATOM | 3084 | CA | ASN | B | 181 | 10.927 | 37.473 | 30.560 | 1.00 | 70.42 | 6 |
| | ATOM | 3085 | CB | ASN | B | 181 | 10.755 | 37.816 | 32.052 | 1.00 | 71.53 | 6 |
| | ATOM | 3086 | CG | ASN | B | 181 | 12.058 | 38.021 | 32.760 | 1.00 | 71.03 | 6 |
| | ATOM | 3087 | OD1 | ASN | B | 181 | 12.935 | 38.731 | 32.267 | 1.00 | 71.52 | 8 |
| | ATOM | 3088 | ND2 | ASN | B | 181 | 12.195 | 37.412 | 33.940 | 1.00 | 71.36 | 7 |
| 40 | ATOM | 3089 | C | ASN | B | 181 | 11.125 | 38.768 | 29.779 | 1.00 | 70.25 | 6 |
| | ATOM | 3090 | O | ASN | B | 181 | 12.104 | 39.478 | 29.975 | 1.00 | 70.25 | 8 |
| | ATOM | 3091 | N | SER | B | 182 | 10.162 | 39.078 | 28.911 | 1.00 | 70.77 | 7 |
| | ATOM | 3092 | CA | SER | B | 182 | 10.203 | 40.297 | 28.105 | 1.00 | 70.64 | 6 |
| | ATOM | 3093 | CB | SER | B | 182 | 9.107 | 40.262 | 27.045 | 1.00 | 70.47 | 6 |
| | ATOM | 3094 | OG | SER | B | 182 | 9.267 | 41.327 | 26.122 | 1.00 | 71.28 | 8 |
| | ATOM | 3095 | C | SER | B | 182 | 9.997 | 41.500 | 29.024 | 1.00 | 70.77 | 6 |
| 45 | ATOM | 3096 | O | SER | B | 182 | 9.429 | 41.359 | 30.095 | 1.00 | 72.80 | 8 |
| | ATOM | 3097 | N | VAL | B | 183 | 10.442 | 42.680 | 28.600 | 1.00 | 71.20 | 7 |
| | ATOM | 3098 | CA | VAL | B | 183 | 10.334 | 43.887 | 29.425 | 1.00 | 70.43 | 6 |
| | ATOM | 3099 | CB | VAL | B | 183 | 11.337 | 43.826 | 30.630 | 1.00 | 68.47 | 6 |
| | ATOM | 3100 | CG1 | VAL | B | 183 | 12.636 | 43.178 | 30.202 | 1.00 | 68.72 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|----------|
| 5 | ATOM | 3101 | CG2 | VAL B 183 | 11.625 | 45.230 | 31.148 | 1.00 | 67.78 6 |
| | ATOM | 3102 | C | VAL B 183 | 10.590 | 45.189 | 28.659 | 1.00 | 70.59 6 |
| | ATOM | 3103 | O | VAL B 183 | 11.522 | 45.282 | 27.853 | 1.00 | 71.25 8 |
| | ATOM | 3104 | N | THR B 184 | 9.761 | 46.195 | 28.911 | 1.00 | 70.21 7 |
| | ATOM | 3105 | CA | THR B 184 | 9.949 | 47.480 | 28.250 | 1.00 | 71.59 6 |
| 10 | ATOM | 3106 | CB | THR B 184 | 8.610 | 48.062 | 27.711 | 1.00 | 70.78 6 |
| | ATOM | 3107 | OG1 | THR B 184 | 8.065 | 47.183 | 26.721 | 1.00 | 69.37 8 |
| | ATOM | 3108 | CG2 | THR B 184 | 8.836 | 49.431 | 27.074 | 1.00 | 69.81 6 |
| | ATOM | 3109 | C | THR B 184 | 10.558 | 48.447 | 29.271 | 1.00 | 73.13 6 |
| | ATOM | 3110 | O | THR B 184 | 10.240 | 48.384 | 30.467 | 1.00 | 73.23 8 |
| 15 | ATOM | 3111 | N | TYR B 185 | 11.449 | 49.319 | 28.806 | 1.00 | 74.37 7 |
| | ATOM | 3112 | CA | TYR B 185 | 12.085 | 50.287 | 29.689 | 1.00 | 76.17 6 |
| | ATOM | 3113 | CB | TYR B 185 | 13.614 | 50.134 | 29.663 | 1.00 | 77.19 6 |
| | ATOM | 3114 | CG | TYR B 185 | 14.076 | 48.723 | 29.912 | 1.00 | 78.36 6 |
| | ATOM | 3115 | CD1 | TYR B 185 | 13.942 | 47.745 | 28.928 | 1.00 | 78.94 6 |
| 20 | ATOM | 3116 | CE1 | TYR B 185 | 14.298 | 46.417 | 29.178 | 1.00 | 80.41 6 |
| | ATOM | 3117 | CD2 | TYR B 185 | 14.584 | 48.344 | 31.154 | 1.00 | 79.09 6 |
| | ATOM | 3118 | CE2 | TYR B 185 | 14.944 | 47.013 | 31.413 | 1.00 | 79.41 6 |
| | ATOM | 3119 | CZ | TYR B 185 | 14.796 | 46.054 | 30.424 | 1.00 | 79.27 6 |
| | ATOM | 3120 | OH | TYR B 185 | 15.119 | 44.731 | 30.677 | 1.00 | 79.15 8 |
| 25 | ATOM | 3121 | C | TYR B 185 | 11.713 | 51.670 | 29.209 | 1.00 | 76.81 6 |
| | ATOM | 3122 | O | TYR B 185 | 11.669 | 51.927 | 28.003 | 1.00 | 76.75 8 |
| | ATOM | 3123 | N | SER B 186 | 11.445 | 52.563 | 30.152 | 1.00 | 78.68 7 |
| | ATOM | 3124 | CA | SER B 186 | 11.078 | 53.941 | 29.810 | 1.00 | 80.00 6 |
| | ATOM | 3125 | CB | SER B 186 | 11.002 | 54.795 | 31.089 | 1.00 | 80.19 6 |
| 30 | ATOM | 3126 | OG | SER B 186 | 12.160 | 54.610 | 31.902 | 1.00 | 79.86 8 |
| | ATOM | 3127 | C | SER B 186 | 12.100 | 54.539 | 28.832 | 1.00 | 80.21 6 |
| | ATOM | 3128 | O | SER B 186 | 11.745 | 55.296 | 27.923 | 1.00 | 79.15 8 |
| | ATOM | 3129 | N | CYS B 187 | 13.364 | 54.171 | 29.025 | 1.00 | 80.45 7 |
| | ATOM | 3130 | CA | CYS B 187 | 14.459 | 54.653 | 28.189 | 1.00 | 80.85 6 |
| 35 | ATOM | 3131 | C | CYS B 187 | 14.259 | 54.260 | 26.772 | 1.00 | 81.01 6 |
| | ATOM | 3132 | O | CYS B 187 | 14.510 | 55.018 | 25.838 | 1.00 | 80.34 8 |
| | ATOM | 3133 | CB | CYS B 187 | 15.787 | 53.993 | 28.574 | 1.00 | 81.53 6 |
| | ATOM | 3134 | SG | CYS B 187 | 15.913 | 52.165 | 28.268 | 1.00 | 84.25 16 |
| | ATOM | 3135 | N | CYS B 188 | 13.791 | 53.035 | 26.637 | 1.00 | 82.80 7 |
| 40 | ATOM | 3136 | CA | CYS B 188 | 13.712 | 52.411 | 25.339 | 1.00 | 83.26 6 |
| | ATOM | 3137 | C | CYS B 188 | 12.352 | 51.851 | 24.849 | 1.00 | 82.46 6 |
| | ATOM | 3138 | O | CYS B 188 | 11.733 | 50.977 | 25.491 | 1.00 | 82.70 8 |
| | ATOM | 3139 | CB | CYS B 188 | 14.811 | 51.336 | 25.365 | 1.00 | 82.41 6 |
| | ATOM | 3140 | SG | CYS B 188 | 16.353 | 51.824 | 26.282 | 1.00 | 83.49 16 |
| 45 | ATOM | 3141 | N | PRO B 189 | 11.891 | 52.346 | 23.679 | 1.00 | 81.48 7 |
| | ATOM | 3142 | CD | PRO B 189 | 12.734 | 53.291 | 22.910 | 1.00 | 81.13 6 |
| | ATOM | 3143 | CA | PRO B 189 | 10.652 | 52.037 | 22.938 | 1.00 | 79.97 6 |
| | ATOM | 3144 | CB | PRO B 189 | 10.977 | 52.510 | 21.517 | 1.00 | 80.12 6 |
| | ATOM | 3145 | CG | PRO B 189 | 11.825 | 53.725 | 21.766 | 1.00 | 80.41 6 |
| 50 | ATOM | 3146 | C | PRO B 189 | 10.133 | 50.585 | 22.941 | 1.00 | 78.77 6 |
| | ATOM | 3147 | O | PRO B 189 | 9.063 | 50.303 | 23.490 | 1.00 | 78.66 8 |
| | ATOM | 3148 | N | GLU B 190 | 10.878 | 49.671 | 22.313 | 1.00 | 77.68 7 |
| | ATOM | 3149 | CA | GLU B 190 | 10.473 | 48.254 | 22.219 | 1.00 | 73.96 6 |
| | ATOM | 3150 | CB | GLU B 190 | 11.214 | 47.570 | 21.075 | 1.00 | 75.24 6 |
| 55 | ATOM | 3151 | CG | GLU B 190 | 11.578 | 48.475 | 19.908 | 1.00 | 77.67 6 |
| | ATOM | 3152 | CD | GLU B 190 | 10.414 | 48.680 | 18.950 | 1.00 | 79.11 6 |
| | ATOM | 3153 | OE1 | GLU B 190 | 9.731 | 47.672 | 18.617 | 1.00 | 77.05 8 |
| | ATOM | 3154 | OE2 | GLU B 190 | 10.200 | 49.845 | 18.526 | 1.00 | 79.84 8 |
| | ATOM | 3155 | C | GLU B 190 | 10.779 | 47.482 | 23.494 | 1.00 | 71.49 6 |
| 60 | ATOM | 3156 | O | GLU B 190 | 11.317 | 48.038 | 24.460 | 1.00 | 71.14 8 |
| | ATOM | 3157 | N | ALA B 191 | 10.455 | 46.191 | 23.483 | 1.00 | 68.33 7 |
| | ATOM | 3158 | CA | ALA B 191 | 10.708 | 45.331 | 24.638 | 1.00 | 66.03 6 |
| | ATOM | 3159 | CB | ALA B 191 | 9.554 | 44.340 | 24.801 | 1.00 | 65.95 6 |
| | ATOM | 3160 | C | ALA B 191 | 12.035 | 44.570 | 24.489 | 1.00 | 64.66 6 |
| | ATOM | 3161 | O | ALA B 191 | 12.439 | 44.225 | 23.374 | 1.00 | 63.36 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3162 | N | TYR | B | 192 | 12.704 | 44.306 | 25.608 | 1.00 | 62.75 | 7 |
| | ATOM | 3163 | CA | TYR | B | 192 | 13.969 | 43.574 | 25.572 | 1.00 | 61.63 | 6 |
| | ATOM | 3164 | CB | TYR | B | 192 | 15.134 | 44.468 | 26.010 | 1.00 | 59.80 | 6 |
| 5 | ATOM | 3165 | CG | TYR | B | 192 | 15.465 | 45.538 | 25.010 | 1.00 | 59.56 | 6 |
| | ATOM | 3166 | CD1 | TYR | B | 192 | 14.786 | 46.754 | 25.005 | 1.00 | 59.46 | 6 |
| | ATOM | 3167 | CE1 | TYR | B | 192 | 15.055 | 47.728 | 24.036 | 1.00 | 60.27 | 6 |
| | ATOM | 3168 | CD2 | TYR | B | 192 | 16.426 | 45.315 | 24.027 | 1.00 | 60.64 | 6 |
| | ATOM | 3169 | CE2 | TYR | B | 192 | 16.705 | 46.274 | 23.057 | 1.00 | 60.97 | 6 |
| | ATOM | 3170 | CZ | TYR | B | 192 | 16.017 | 47.480 | 23.064 | 1.00 | 61.60 | 6 |
| 10 | ATOM | 3171 | OH | TYR | B | 192 | 16.290 | 48.431 | 22.101 | 1.00 | 60.81 | 8 |
| | ATOM | 3172 | C | TYR | B | 192 | 13.948 | 42.302 | 26.426 | 1.00 | 62.58 | 6 |
| | ATOM | 3173 | O | TYR | B | 192 | 14.047 | 42.349 | 27.668 | 1.00 | 62.03 | 8 |
| | ATOM | 3174 | N | GLU | B | 193 | 13.834 | 41.166 | 25.738 | 1.00 | 62.66 | 7 |
| | ATOM | 3175 | CA | GLU | B | 193 | 13.794 | 39.852 | 26.384 | 1.00 | 62.77 | 6 |
| 15 | ATOM | 3176 | CB | GLU | B | 193 | 13.521 | 38.742 | 25.352 | 1.00 | 61.29 | 6 |
| | ATOM | 3177 | CG | GLU | B | 193 | 12.153 | 38.831 | 24.681 | 1.00 | 61.98 | 6 |
| | ATOM | 3178 | CD | GLU | B | 193 | 11.858 | 37.636 | 23.775 | 1.00 | 62.41 | 6 |
| | ATOM | 3179 | OE1 | GLU | B | 193 | 12.059 | 36.486 | 24.228 | 1.00 | 62.14 | 8 |
| | ATOM | 3180 | OE2 | GLU | B | 193 | 11.411 | 37.838 | 22.621 | 1.00 | 62.38 | 8 |
| 20 | ATOM | 3181 | C | GLU | B | 193 | 15.105 | 39.552 | 27.091 | 1.00 | 61.37 | 6 |
| | ATOM | 3182 | O | GLU | B | 193 | 16.166 | 40.019 | 26.666 | 1.00 | 63.09 | 8 |
| | ATOM | 3183 | N | ASP | B | 194 | 15.026 | 38.772 | 28.165 | 1.00 | 58.46 | 7 |
| | ATOM | 3184 | CA | ASP | B | 194 | 16.207 | 38.395 | 28.914 | 1.00 | 57.68 | 6 |
| | ATOM | 3185 | CB | ASP | B | 194 | 16.699 | 39.560 | 29.794 | 1.00 | 58.80 | 6 |
| 25 | ATOM | 3186 | CG | ASP | B | 194 | 15.806 | 39.809 | 31.006 | 1.00 | 61.20 | 6 |
| | ATOM | 3187 | OD1 | ASP | B | 194 | 15.115 | 40.864 | 31.030 | 1.00 | 63.41 | 8 |
| | ATOM | 3188 | OD2 | ASP | B | 194 | 15.804 | 38.955 | 31.930 | 1.00 | 59.40 | 8 |
| | ATOM | 3189 | C | ASP | B | 194 | 15.914 | 37.177 | 29.772 | 1.00 | 56.01 | 6 |
| | ATOM | 3190 | O | ASP | B | 194 | 14.789 | 36.956 | 30.171 | 1.00 | 55.53 | 8 |
| 30 | ATOM | 3191 | N | VAL | B | 195 | 16.943 | 36.385 | 30.036 | 1.00 | 55.28 | 7 |
| | ATOM | 3192 | CA | VAL | B | 195 | 16.819 | 35.199 | 30.860 | 1.00 | 54.79 | 6 |
| | ATOM | 3193 | CB | VAL | B | 195 | 17.662 | 34.053 | 30.300 | 1.00 | 53.86 | 6 |
| | ATOM | 3194 | CG1 | VAL | B | 195 | 17.695 | 32.895 | 31.285 | 1.00 | 51.98 | 6 |
| | ATOM | 3195 | CG2 | VAL | B | 195 | 17.112 | 33.631 | 28.968 | 1.00 | 53.24 | 6 |
| 35 | ATOM | 3196 | C | VAL | B | 195 | 17.334 | 35.522 | 32.248 | 1.00 | 56.42 | 6 |
| | ATOM | 3197 | O | VAL | B | 195 | 18.451 | 36.003 | 32.407 | 1.00 | 58.47 | 8 |
| | ATOM | 3198 | N | GLU | B | 196 | 16.525 | 35.261 | 33.261 | 1.00 | 58.06 | 7 |
| | ATOM | 3199 | CA | GLU | B | 196 | 16.942 | 35.526 | 34.624 | 1.00 | 58.06 | 6 |
| | ATOM | 3200 | CB | GLU | B | 196 | 15.808 | 36.168 | 35.393 | 1.00 | 59.44 | 6 |
| 40 | ATOM | 3201 | CG | GLU | B | 196 | 16.168 | 36.535 | 36.811 | 1.00 | 64.02 | 6 |
| | ATOM | 3202 | CD | GLU | B | 196 | 14.983 | 37.131 | 37.561 | 1.00 | 65.27 | 6 |
| | ATOM | 3203 | OE1 | GLU | B | 196 | 14.414 | 38.137 | 37.081 | 1.00 | 65.41 | 8 |
| | ATOM | 3204 | OE2 | GLU | B | 196 | 14.625 | 36.591 | 38.631 | 1.00 | 68.06 | 8 |
| | ATOM | 3205 | C | GLU | B | 196 | 17.310 | 34.199 | 35.252 | 1.00 | 57.73 | 6 |
| 45 | ATOM | 3206 | O | GLU | B | 196 | 16.495 | 33.285 | 35.291 | 1.00 | 60.64 | 8 |
| | ATOM | 3207 | N | VAL | B | 197 | 18.543 | 34.084 | 35.722 | 1.00 | 56.14 | 7 |
| | ATOM | 3208 | CA | VAL | B | 197 | 18.999 | 32.854 | 36.338 | 1.00 | 54.69 | 6 |
| | ATOM | 3209 | CB | VAL | B | 197 | 20.358 | 32.405 | 35.757 | 1.00 | 52.53 | 6 |
| | ATOM | 3210 | CG1 | VAL | B | 197 | 20.807 | 31.107 | 36.404 | 1.00 | 50.11 | 6 |
| 50 | ATOM | 3211 | CG2 | VAL | B | 197 | 20.241 | 32.229 | 34.264 | 1.00 | 51.73 | 6 |
| | ATOM | 3212 | C | VAL | B | 197 | 19.154 | 33.106 | 37.819 | 1.00 | 56.80 | 6 |
| | ATOM | 3213 | O | VAL | B | 197 | 19.817 | 34.057 | 38.226 | 1.00 | 57.91 | 8 |
| | ATOM | 3214 | N | SER | B | 198 | 18.539 | 32.258 | 38.631 | 1.00 | 58.59 | 7 |
| | ATOM | 3215 | CA | SER | B | 198 | 18.626 | 32.421 | 40.071 | 1.00 | 58.65 | 6 |
| 55 | ATOM | 3216 | CB | SER | B | 198 | 17.235 | 32.308 | 40.703 | 1.00 | 59.34 | 6 |
| | ATOM | 3217 | OG | SER | B | 198 | 16.426 | 33.407 | 40.320 | 1.00 | 59.29 | 8 |
| | ATOM | 3218 | C | SER | B | 198 | 19.556 | 31.385 | 40.651 | 1.00 | 57.58 | 6 |
| | ATOM | 3219 | O | SER | B | 198 | 19.340 | 30.188 | 40.505 | 1.00 | 58.41 | 8 |
| | ATOM | 3220 | N | LEU | B | 199 | 20.599 | 31.857 | 41.310 | 1.00 | 57.49 | 7 |
| 60 | ATOM | 3221 | CA | LEU | B | 199 | 21.569 | 30.963 | 41.904 | 1.00 | 58.89 | 6 |
| | ATOM | 3222 | CB | LEU | B | 199 | 23.000 | 31.437 | 41.622 | 1.00 | 58.76 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3223 | CG | LEU | B | 199 | 24.108 | 30.670 | 42.358 | 1.00 | 59.80 | 6 |
| | ATOM | 3224 | CD1 | LEU | B | 199 | 24.135 | 29.209 | 41.927 | 1.00 | 60.58 | 6 |
| | ATOM | 3225 | CD2 | LEU | B | 199 | 25.446 | 31.304 | 42.063 | 1.00 | 60.42 | 6 |
| | ATOM | 3226 | C | LEU | B | 199 | 21.369 | 30.885 | 43.395 | 1.00 | 60.51 | 6 |
| 5 | ATOM | 3227 | O | LEU | B | 199 | 21.759 | 31.788 | 44.136 | 1.00 | 61.67 | 8 |
| | ATOM | 3228 | N | ASN | B | 200 | 20.754 | 29.801 | 43.838 | 1.00 | 60.15 | 7 |
| | ATOM | 3229 | CA | ASN | B | 200 | 20.539 | 29.607 | 45.252 | 1.00 | 57.57 | 6 |
| | ATOM | 3230 | CB | ASN | B | 200 | 19.188 | 28.919 | 45.499 | 1.00 | 60.95 | 6 |
| | ATOM | 3231 | CG | ASN | B | 200 | 18.936 | 28.642 | 46.968 | 1.00 | 62.80 | 6 |
| 10 | ATOM | 3232 | OD1 | ASN | B | 200 | 19.167 | 29.504 | 47.820 | 1.00 | 65.10 | 8 |
| | ATOM | 3233 | ND2 | ASN | B | 200 | 18.465 | 27.443 | 47.275 | 1.00 | 59.90 | 7 |
| | ATOM | 3234 | C | ASN | B | 200 | 21.691 | 28.736 | 45.712 | 1.00 | 55.80 | 6 |
| | ATOM | 3235 | O | ASN | B | 200 | 21.793 | 27.569 | 45.325 | 1.00 | 56.54 | 8 |
| | ATOM | 3236 | N | PHE | B | 201 | 22.561 | 29.316 | 46.527 | 1.00 | 53.98 | 7 |
| 15 | ATOM | 3237 | CA | PHE | B | 201 | 23.725 | 28.615 | 47.042 | 1.00 | 53.98 | 6 |
| | ATOM | 3238 | CB | PHE | B | 201 | 24.960 | 28.975 | 46.226 | 1.00 | 53.35 | 6 |
| | ATOM | 3239 | CG | PHE | B | 201 | 25.418 | 30.404 | 46.418 | 1.00 | 51.26 | 6 |
| | ATOM | 3240 | CD1 | PHE | B | 201 | 26.633 | 30.690 | 47.050 | 1.00 | 50.15 | 6 |
| | ATOM | 3241 | CD2 | PHE | B | 201 | 24.615 | 31.472 | 46.000 | 1.00 | 50.67 | 6 |
| 20 | ATOM | 3242 | CE1 | PHE | B | 201 | 27.038 | 32.015 | 47.264 | 1.00 | 45.58 | 6 |
| | ATOM | 3243 | CE2 | PHE | B | 201 | 25.016 | 32.799 | 46.213 | 1.00 | 47.69 | 6 |
| | ATOM | 3244 | CZ | PHE | B | 201 | 26.227 | 33.062 | 46.845 | 1.00 | 46.26 | 6 |
| | ATOM | 3245 | C | PHE | B | 201 | 23.943 | 29.080 | 48.456 | 1.00 | 55.95 | 6 |
| | ATOM | 3246 | O | PHE | B | 201 | 23.275 | 30.017 | 48.912 | 1.00 | 56.39 | 8 |
| 25 | ATOM | 3247 | N | ARG | B | 202 | 24.896 | 28.443 | 49.132 | 1.00 | 56.81 | 7 |
| | ATOM | 3248 | CA | ARG | B | 202 | 25.223 | 28.793 | 50.506 | 1.00 | 60.77 | 6 |
| | ATOM | 3249 | CB | ARG | B | 202 | 24.255 | 28.104 | 51.460 | 1.00 | 64.25 | 6 |
| | ATOM | 3250 | CG | ARG | B | 202 | 24.491 | 26.625 | 51.497 | 1.00 | 66.78 | 6 |
| | ATOM | 3251 | CD | ARG | B | 202 | 23.494 | 25.893 | 52.344 | 1.00 | 70.08 | 6 |
| 30 | ATOM | 3252 | NE | ARG | B | 202 | 23.768 | 24.454 | 52.333 | 1.00 | 72.69 | 7 |
| | ATOM | 3253 | CZ | ARG | B | 202 | 22.945 | 23.528 | 52.825 | 1.00 | 73.67 | 6 |
| | ATOM | 3254 | NH1 | ARG | B | 202 | 21.781 | 23.884 | 53.375 | 1.00 | 74.01 | 7 |
| | ATOM | 3255 | NH2 | ARG | B | 202 | 23.281 | 22.245 | 52.760 | 1.00 | 73.29 | 7 |
| | ATOM | 3256 | C | ARG | B | 202 | 26.635 | 28.328 | 50.843 | 1.00 | 61.67 | 6 |
| 35 | ATOM | 3257 | O | ARG | B | 202 | 27.181 | 27.450 | 50.183 | 1.00 | 62.10 | 8 |
| | ATOM | 3258 | N | LYS | B | 203 | 27.225 | 28.918 | 51.875 | 1.00 | 62.58 | 7 |
| | ATOM | 3259 | CA | LYS | B | 203 | 28.549 | 28.505 | 52.298 | 1.00 | 62.87 | 6 |
| | ATOM | 3260 | CB | LYS | B | 203 | 29.067 | 29.417 | 53.399 | 1.00 | 62.83 | 6 |
| | ATOM | 3261 | CG | LYS | B | 203 | 30.400 | 28.995 | 53.967 | 1.00 | 62.29 | 6 |
| 40 | ATOM | 3262 | CD | LYS | B | 203 | 30.765 | 29.871 | 55.141 | 1.00 | 65.39 | 6 |
| | ATOM | 3263 | CE | LYS | B | 203 | 32.135 | 29.519 | 55.689 | 1.00 | 67.38 | 6 |
| | ATOM | 3264 | NZ | LYS | B | 203 | 33.232 | 29.772 | 54.695 | 1.00 | 70.43 | 7 |
| | ATOM | 3265 | C | LYS | B | 203 | 28.387 | 27.101 | 52.854 | 1.00 | 64.30 | 6 |
| | ATOM | 3266 | O | LYS | B | 203 | 27.318 | 26.736 | 53.371 | 1.00 | 65.43 | 8 |
| 45 | ATOM | 3267 | N | LYS | B | 204 | 29.446 | 26.312 | 52.745 | 1.00 | 66.12 | 7 |
| | ATOM | 3268 | CA | LYS | B | 204 | 29.417 | 24.955 | 53.246 | 1.00 | 67.10 | 6 |
| | ATOM | 3269 | CB | LYS | B | 204 | 30.701 | 24.223 | 52.860 | 1.00 | 63.37 | 6 |
| | ATOM | 3270 | CG | LYS | B | 204 | 30.745 | 23.853 | 51.379 | 1.00 | 60.21 | 6 |
| | ATOM | 3271 | CD | LYS | B | 204 | 31.940 | 22.966 | 51.055 | 1.00 | 58.61 | 6 |
| 50 | ATOM | 3272 | CE | LYS | B | 204 | 31.955 | 22.553 | 49.582 | 1.00 | 57.79 | 6 |
| | ATOM | 3273 | NZ | LYS | B | 204 | 33.202 | 21.808 | 49.238 | 1.00 | 53.82 | 7 |
| | ATOM | 3274 | C | LYS | B | 204 | 29.293 | 25.081 | 54.745 | 1.00 | 70.90 | 6 |
| | ATOM | 3275 | O | LYS | B | 204 | 29.893 | 25.989 | 55.339 | 1.00 | 72.60 | 8 |
| | ATOM | 3276 | N | GLY | B | 205 | 28.489 | 24.192 | 55.342 | 1.00 | 74.01 | 7 |
| 55 | ATOM | 3277 | CA | GLY | B | 205 | 28.260 | 24.197 | 56.783 | 1.00 | 74.37 | 6 |
| | ATOM | 3278 | C | GLY | B | 205 | 29.305 | 23.430 | 57.576 | 1.00 | 75.59 | 6 |
| | ATOM | 3279 | OT1 | GLY | B | 205 | 30.276 | 22.932 | 56.958 | 1.00 | 75.56 | 8 |
| | ATOM | 3280 | OT2 | GLY | B | 205 | 29.163 | 23.331 | 58.822 | 1.00 | 76.47 | 8 |
| | ATOM | 3281 | CB | PHE | C | 1 | 16.639 | 48.183 | 2.177 | 1.00 | 71.30 | 6 |
| 60 | ATOM | 3282 | CG | PHE | C | 1 | 17.365 | 49.162 | 1.297 | 1.00 | 73.66 | 6 |
| | ATOM | 3283 | CD1 | PHE | C | 1 | 18.546 | 48.805 | 0.647 | 1.00 | 74.99 | 6 |

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|----|------|------|-----|-----|---|---|--------|--------|--------|------|-------|---|
| | ATOM | 3284 | CD2 | PHE | C | 1 | 16.889 | 50.471 | 1.160 | 1.00 | 75.46 | 6 |
| | ATOM | 3285 | CE1 | PHE | C | 1 | 19.257 | 49.743 | -0.138 | 1.00 | 77.68 | 6 |
| | ATOM | 3286 | CE2 | PHE | C | 1 | 17.590 | 51.421 | 0.380 | 1.00 | 76.94 | 6 |
| | ATOM | 3287 | CZ | PHE | C | 1 | 18.779 | 51.054 | -0.271 | 1.00 | 77.37 | 6 |
| 5 | ATOM | 3288 | C | PHE | C | 1 | 16.469 | 45.841 | 2.896 | 1.00 | 69.30 | 6 |
| | ATOM | 3289 | O | PHE | C | 1 | 15.487 | 45.976 | 3.637 | 1.00 | 68.12 | 8 |
| | ATOM | 3290 | N | PHE | C | 1 | 15.624 | 46.515 | 0.608 | 1.00 | 67.59 | 7 |
| | ATOM | 3291 | CA | PHE | C | 1 | 16.651 | 46.733 | 1.669 | 1.00 | 69.36 | 6 |
| | ATOM | 3292 | N | ASP | C | 2 | 17.421 | 44.940 | 3.123 | 1.00 | 69.61 | 7 |
| 10 | ATOM | 3293 | CA | ASP | C | 2 | 17.373 | 44.071 | 4.298 | 1.00 | 68.32 | 6 |
| | ATOM | 3294 | CB | ASP | C | 2 | 17.364 | 42.592 | 3.882 | 1.00 | 69.98 | 6 |
| | ATOM | 3295 | CG | ASP | C | 2 | 18.729 | 42.092 | 3.426 | 1.00 | 71.56 | 6 |
| | ATOM | 3296 | OD1 | ASP | C | 2 | 19.586 | 41.867 | 4.316 | 1.00 | 71.73 | 8 |
| | ATOM | 3297 | OD2 | ASP | C | 2 | 18.936 | 41.926 | 2.187 | 1.00 | 72.36 | 8 |
| 15 | ATOM | 3298 | C | ASP | C | 2 | 18.615 | 44.399 | 5.116 | 1.00 | 66.00 | 6 |
| | ATOM | 3299 | O | ASP | C | 2 | 19.617 | 44.865 | 4.562 | 1.00 | 67.56 | 8 |
| | ATOM | 3300 | N | ARG | C | 3 | 18.550 | 44.165 | 6.423 | 1.00 | 62.29 | 7 |
| | ATOM | 3301 | CA | ARG | C | 3 | 19.663 | 44.455 | 7.320 | 1.00 | 59.37 | 6 |
| | ATOM | 3302 | CB | ARG | C | 3 | 19.515 | 43.661 | 8.604 | 1.00 | 56.89 | 6 |
| 20 | ATOM | 3303 | CG | ARG | C | 3 | 18.280 | 44.017 | 9.387 | 1.00 | 55.35 | 6 |
| | ATOM | 3304 | CD | ARG | C | 3 | 18.177 | 43.172 | 10.640 | 1.00 | 57.70 | 6 |
| | ATOM | 3305 | NE | ARG | C | 3 | 16.947 | 43.437 | 11.378 | 1.00 | 60.36 | 7 |
| | ATOM | 3306 | CZ | ARG | C | 3 | 16.714 | 44.540 | 12.084 | 1.00 | 62.92 | 6 |
| | ATOM | 3307 | NH1 | ARG | C | 3 | 17.623 | 45.503 | 12.166 | 1.00 | 62.53 | 7 |
| 25 | ATOM | 3308 | NH2 | ARG | C | 3 | 15.554 | 44.689 | 12.700 | 1.00 | 64.87 | 7 |
| | ATOM | 3309 | C | ARG | C | 3 | 21.060 | 44.236 | 6.749 | 1.00 | 59.30 | 6 |
| | ATOM | 3310 | O | ARG | C | 3 | 21.970 | 45.008 | 7.051 | 1.00 | 61.36 | 8 |
| | ATOM | 3311 | N | ALA | C | 4 | 21.257 | 43.215 | 5.920 | 1.00 | 57.54 | 7 |
| | ATOM | 3312 | CA | ALA | C | 4 | 22.595 | 43.023 | 5.379 | 1.00 | 55.37 | 6 |
| 30 | ATOM | 3313 | CB | ALA | C | 4 | 22.686 | 41.727 | 4.610 | 1.00 | 53.55 | 6 |
| | ATOM | 3314 | C | ALA | C | 4 | 22.947 | 44.186 | 4.478 | 1.00 | 54.97 | 6 |
| | ATOM | 3315 | O | ALA | C | 4 | 24.020 | 44.764 | 4.603 | 1.00 | 55.12 | 8 |
| | ATOM | 3316 | N | ASP | C | 5 | 22.034 | 44.534 | 3.575 | 1.00 | 56.24 | 7 |
| | ATOM | 3317 | CA | ASP | C | 5 | 22.265 | 45.632 | 2.646 | 1.00 | 56.25 | 6 |
| 35 | ATOM | 3318 | CB | ASP | C | 5 | 21.081 | 45.795 | 1.680 | 1.00 | 58.72 | 6 |
| | ATOM | 3319 | CG | ASP | C | 5 | 20.773 | 44.529 | 0.906 | 1.00 | 62.35 | 6 |
| | ATOM | 3320 | OD1 | ASP | C | 5 | 21.715 | 43.900 | 0.364 | 1.00 | 63.21 | 8 |
| | ATOM | 3321 | OD2 | ASP | C | 5 | 19.574 | 44.171 | 0.834 | 1.00 | 65.38 | 8 |
| | ATOM | 3322 | C | ASP | C | 5 | 22.471 | 46.935 | 3.406 | 1.00 | 55.27 | 6 |
| 40 | ATOM | 3323 | O | ASP | C | 5 | 23.294 | 47.764 | 3.020 | 1.00 | 54.31 | 8 |
| | ATOM | 3324 | N | ILE | C | 6 | 21.732 | 47.110 | 4.495 | 1.00 | 53.55 | 7 |
| | ATOM | 3325 | CA | ILE | C | 6 | 21.840 | 48.339 | 5.270 | 1.00 | 54.16 | 6 |
| | ATOM | 3326 | CB | ILE | C | 6 | 20.713 | 48.456 | 6.311 | 1.00 | 54.45 | 6 |
| | ATOM | 3327 | CG2 | ILE | C | 6 | 20.811 | 49.793 | 7.021 | 1.00 | 52.65 | 6 |
| 45 | ATOM | 3328 | CG1 | ILE | C | 6 | 19.352 | 48.344 | 5.612 | 1.00 | 56.53 | 6 |
| | ATOM | 3329 | CD1 | ILE | C | 6 | 18.146 | 48.530 | 6.524 | 1.00 | 56.74 | 6 |
| | ATOM | 3330 | C | ILE | C | 6 | 23.178 | 48.475 | 5.972 | 1.00 | 52.95 | 6 |
| | ATOM | 3331 | O | ILE | C | 6 | 23.872 | 49.487 | 5.818 | 1.00 | 53.74 | 8 |
| | ATOM | 3332 | N | LEU | C | 7 | 23.543 | 47.455 | 6.741 | 1.00 | 51.30 | 7 |
| 50 | ATOM | 3333 | CA | LEU | C | 7 | 24.814 | 47.462 | 7.460 | 1.00 | 49.62 | 6 |
| | ATOM | 3334 | CB | LEU | C | 7 | 24.931 | 46.194 | 8.293 | 1.00 | 47.45 | 6 |
| | ATOM | 3335 | CG | LEU | C | 7 | 23.912 | 46.136 | 9.429 | 1.00 | 47.62 | 6 |
| | ATOM | 3336 | CD1 | LEU | C | 7 | 23.819 | 44.743 | 10.014 | 1.00 | 48.73 | 6 |
| | ATOM | 3337 | CD2 | LEU | C | 7 | 24.321 | 47.122 | 10.486 | 1.00 | 47.41 | 6 |
| 55 | ATOM | 3338 | C | LEU | C | 7 | 25.970 | 47.559 | 6.465 | 1.00 | 49.71 | 6 |
| | ATOM | 3339 | O | LEU | C | 7 | 26.951 | 48.269 | 6.677 | 1.00 | 47.57 | 8 |
| | ATOM | 3340 | N | TYR | C | 8 | 25.827 | 46.845 | 5.361 | 1.00 | 52.00 | 7 |
| | ATOM | 3341 | CA | TYR | C | 8 | 26.830 | 46.838 | 4.318 | 1.00 | 53.34 | 6 |
| | ATOM | 3342 | CB | TYR | C | 8 | 26.367 | 45.961 | 3.167 | 1.00 | 53.82 | 6 |
| 60 | ATOM | 3343 | CG | TYR | C | 8 | 27.335 | 45.969 | 2.020 | 1.00 | 57.66 | 6 |
| | ATOM | 3344 | CD1 | TYR | C | 8 | 28.552 | 45.289 | 2.106 | 1.00 | 58.72 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3345 | CE1 | TYR | C | 8 | 29.467 | 45.315 | 1.045 | 1.00 | 60.33 | 6 |
| | ATOM | 3346 | CD2 | TYR | C | 8 | 27.051 | 46.679 | 0.851 | 1.00 | 58.73 | 6 |
| | ATOM | 3347 | CE2 | TYR | C | 8 | 27.957 | 46.714 | -0.211 | 1.00 | 60.05 | 6 |
| | ATOM | 3348 | CZ | TYR | C | 8 | 29.162 | 46.027 | -0.107 | 1.00 | 60.68 | 6 |
| 5 | ATOM | 3349 | OH | TYR | C | 8 | 30.045 | 46.045 | -1.163 | 1.00 | 62.86 | 8 |
| | ATOM | 3350 | C | TYR | C | 8 | 27.134 | 48.235 | 3.790 | 1.00 | 54.25 | 6 |
| | ATOM | 3351 | O | TYR | C | 8 | 28.298 | 48.589 | 3.614 | 1.00 | 55.00 | 8 |
| | ATOM | 3352 | N | ASN | C | 9 | 26.092 | 49.015 | 3.516 | 1.00 | 53.76 | 7 |
| | ATOM | 3353 | CA | ASN | C | 9 | 26.283 | 50.369 | 3.013 | 1.00 | 55.35 | 6 |
| 10 | ATOM | 3354 | CB | ASN | C | 9 | 24.941 | 51.005 | 2.660 | 1.00 | 59.27 | 6 |
| | ATOM | 3355 | CG | ASN | C | 9 | 24.299 | 50.372 | 1.433 | 1.00 | 61.31 | 6 |
| | ATOM | 3356 | OD1 | ASN | C | 9 | 24.907 | 49.531 | 0.758 | 1.00 | 61.18 | 8 |
| | ATOM | 3357 | ND2 | ASN | C | 9 | 23.068 | 50.778 | 1.136 | 1.00 | 62.69 | 7 |
| | ATOM | 3358 | C | ASN | C | 9 | 27.003 | 51.233 | 4.034 | 1.00 | 54.14 | 6 |
| 15 | ATOM | 3359 | O | ASN | C | 9 | 28.001 | 51.877 | 3.722 | 1.00 | 54.09 | 8 |
| | ATOM | 3360 | N | ILE | C | 10 | 26.494 | 51.240 | 5.258 | 1.00 | 54.05 | 7 |
| | ATOM | 3361 | CA | ILE | C | 10 | 27.107 | 52.014 | 6.330 | 1.00 | 54.35 | 6 |
| | ATOM | 3362 | CB | ILE | C | 10 | 26.399 | 51.757 | 7.668 | 1.00 | 53.88 | 6 |
| | ATOM | 3363 | CG2 | ILE | C | 10 | 27.141 | 52.453 | 8.784 | 1.00 | 52.27 | 6 |
| 20 | ATOM | 3364 | CG1 | ILE | C | 10 | 24.956 | 52.257 | 7.595 | 1.00 | 53.43 | 6 |
| | ATOM | 3365 | CD1 | ILE | C | 10 | 24.114 | 51.860 | 8.769 | 1.00 | 51.08 | 6 |
| | ATOM | 3366 | C | ILE | C | 10 | 28.580 | 51.635 | 6.479 | 1.00 | 55.70 | 6 |
| | ATOM | 3367 | O | ILE | C | 10 | 29.452 | 52.497 | 6.609 | 1.00 | 56.88 | 8 |
| | ATOM | 3368 | N | ARG | C | 11 | 28.844 | 50.337 | 6.456 | 1.00 | 56.11 | 7 |
| 25 | ATOM | 3369 | CA | ARG | C | 11 | 30.194 | 49.827 | 6.579 | 1.00 | 57.74 | 6 |
| | ATOM | 3370 | CB | ARG | C | 11 | 30.161 | 48.307 | 6.466 | 1.00 | 61.80 | 6 |
| | ATOM | 3371 | CG | ARG | C | 11 | 31.495 | 47.629 | 6.644 | 1.00 | 67.28 | 6 |
| | ATOM | 3372 | CD | ARG | C | 11 | 31.879 | 47.631 | 8.102 | 1.00 | 75.61 | 6 |
| | ATOM | 3373 | NE | ARG | C | 11 | 32.848 | 46.586 | 8.419 | 1.00 | 82.91 | 7 |
| 30 | ATOM | 3374 | CZ | ARG | C | 11 | 32.779 | 45.333 | 7.957 | 1.00 | 86.49 | 6 |
| | ATOM | 3375 | NH1 | ARG | C | 11 | 31.785 | 44.963 | 7.140 | 1.00 | 87.62 | 7 |
| | ATOM | 3376 | NH2 | ARG | C | 11 | 33.689 | 44.436 | 8.331 | 1.00 | 87.96 | 7 |
| | ATOM | 3377 | C | ARG | C | 11 | 31.099 | 50.388 | 5.490 | 1.00 | 57.06 | 6 |
| | ATOM | 3378 | O | ARG | C | 11 | 32.198 | 50.865 | 5.758 | 1.00 | 57.56 | 8 |
| 35 | ATOM | 3379 | N | GLN | C | 12 | 30.617 | 50.333 | 4.255 | 1.00 | 57.22 | 7 |
| | ATOM | 3380 | CA | GLN | C | 12 | 31.377 | 50.781 | 3.093 | 1.00 | 56.59 | 6 |
| | ATOM | 3381 | CB | GLN | C | 12 | 30.783 | 50.169 | 1.829 | 1.00 | 56.62 | 6 |
| | ATOM | 3382 | CG | GLN | C | 12 | 31.795 | 49.448 | 0.976 | 1.00 | 58.01 | 6 |
| | ATOM | 3383 | CD | GLN | C | 12 | 32.113 | 48.101 | 1.532 | 1.00 | 58.10 | 6 |
| 40 | ATOM | 3384 | OE1 | GLN | C | 12 | 31.215 | 47.289 | 1.704 | 1.00 | 59.91 | 8 |
| | ATOM | 3385 | NE2 | GLN | C | 12 | 33.384 | 47.846 | 1.824 | 1.00 | 57.19 | 7 |
| | ATOM | 3386 | C | GLN | C | 12 | 31.505 | 52.278 | 2.872 | 1.00 | 56.02 | 6 |
| | ATOM | 3387 | O | GLN | C | 12 | 32.424 | 52.728 | 2.208 | 1.00 | 54.27 | 8 |
| | ATOM | 3388 | N | THR | C | 13 | 30.589 | 53.054 | 3.423 | 1.00 | 58.04 | 7 |
| 45 | ATOM | 3389 | CA | THR | C | 13 | 30.631 | 54.492 | 3.213 | 1.00 | 59.72 | 6 |
| | ATOM | 3390 | CB | THR | C | 13 | 29.302 | 54.985 | 2.653 | 1.00 | 58.83 | 6 |
| | ATOM | 3391 | OG1 | THR | C | 13 | 28.253 | 54.622 | 3.559 | 1.00 | 55.46 | 8 |
| | ATOM | 3392 | CG2 | THR | C | 13 | 29.043 | 54.374 | 1.277 | 1.00 | 59.29 | 6 |
| | ATOM | 3393 | C | THR | C | 13 | 30.944 | 55.316 | 4.459 | 1.00 | 61.81 | 6 |
| 50 | ATOM | 3394 | O | THR | C | 13 | 31.317 | 56.492 | 4.364 | 1.00 | 62.06 | 8 |
| | ATOM | 3395 | N | SER | C | 14 | 30.794 | 54.705 | 5.627 | 1.00 | 62.55 | 7 |
| | ATOM | 3396 | CA | SER | C | 14 | 31.053 | 55.421 | 6.865 | 1.00 | 62.19 | 6 |
| | ATOM | 3397 | CB | SER | C | 14 | 30.549 | 54.612 | 8.056 | 1.00 | 62.76 | 6 |
| | ATOM | 3398 | OG | SER | C | 14 | 30.476 | 55.435 | 9.209 | 1.00 | 64.16 | 8 |
| 55 | ATOM | 3399 | C | SER | C | 14 | 32.521 | 55.779 | 7.074 | 1.00 | 61.03 | 6 |
| | ATOM | 3400 | O | SER | C | 14 | 33.422 | 55.098 | 6.577 | 1.00 | 61.70 | 8 |
| | ATOM | 3401 | N | ARG | C | 15 | 32.735 | 56.863 | 7.816 | 1.00 | 58.93 | 7 |
| | ATOM | 3402 | CA | ARG | C | 15 | 34.064 | 57.367 | 8.127 | 1.00 | 57.11 | 6 |
| | ATOM | 3403 | CB | ARG | C | 15 | 34.383 | 58.576 | 7.247 | 1.00 | 57.80 | 6 |
| 60 | ATOM | 3404 | CG | ARG | C | 15 | 34.388 | 58.261 | 5.748 | 1.00 | 59.34 | 6 |
| | ATOM | 3405 | CD | ARG | C | 15 | 35.114 | 59.331 | 4.968 | 1.00 | 61.90 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3406 | NE | ARG | C | 15 | 36.475 | 59.479 | 5.475 | 1.00 | 64.09 | 7 |
| | ATOM | 3407 | CZ | ARG | C | 15 | 37.287 | 60.488 | 5.180 | 1.00 | 63.60 | 6 |
| | ATOM | 3408 | NH1 | ARG | C | 15 | 36.873 | 61.450 | 4.375 | 1.00 | 62.16 | 7 |
| | ATOM | 3409 | NH2 | ARG | C | 15 | 38.516 | 60.526 | 5.688 | 1.00 | 66.26 | 7 |
| 5 | ATOM | 3410 | C | ARG | C | 15 | 34.081 | 57.753 | 9.598 | 1.00 | 54.80 | 6 |
| | ATOM | 3411 | O | ARG | C | 15 | 33.736 | 58.874 | 9.969 | 1.00 | 54.31 | 8 |
| | ATOM | 3412 | N | PRO | C | 16 | 34.483 | 56.811 | 10.460 | 1.00 | 53.16 | 7 |
| | ATOM | 3413 | CD | PRO | C | 16 | 34.921 | 55.451 | 10.106 | 1.00 | 49.32 | 6 |
| | ATOM | 3414 | CA | PRO | C | 16 | 34.547 | 57.012 | 11.911 | 1.00 | 51.93 | 6 |
| 10 | ATOM | 3415 | CB | PRO | C | 16 | 35.072 | 55.668 | 12.429 | 1.00 | 49.26 | 6 |
| | ATOM | 3416 | CG | PRO | C | 16 | 34.647 | 54.702 | 11.387 | 1.00 | 48.93 | 6 |
| | ATOM | 3417 | C | PRO | C | 16 | 35.420 | 58.172 | 12.356 | 1.00 | 51.62 | 6 |
| | ATOM | 3418 | O | PRO | C | 16 | 35.266 | 58.663 | 13.468 | 1.00 | 52.27 | 8 |
| | ATOM | 3419 | N | ASP | C | 17 | 36.337 | 58.608 | 11.501 | 1.00 | 51.78 | 7 |
| 15 | ATOM | 3420 | CA | ASP | C | 17 | 37.219 | 59.706 | 11.863 | 1.00 | 54.16 | 6 |
| | ATOM | 3421 | CB | ASP | C | 17 | 38.597 | 59.526 | 11.209 | 1.00 | 59.36 | 6 |
| | ATOM | 3422 | CG | ASP | C | 17 | 39.421 | 58.411 | 11.859 | 1.00 | 64.02 | 6 |
| | ATOM | 3423 | OD1 | ASP | C | 17 | 39.200 | 58.134 | 13.067 | 1.00 | 64.61 | 8 |
| | ATOM | 3424 | OD2 | ASP | C | 17 | 40.299 | 57.824 | 11.170 | 1.00 | 64.76 | 8 |
| 20 | ATOM | 3425 | C | ASP | C | 17 | 36.680 | 61.080 | 11.499 | 1.00 | 53.77 | 6 |
| | ATOM | 3426 | O | ASP | C | 17 | 37.350 | 62.088 | 11.736 | 1.00 | 54.82 | 8 |
| | ATOM | 3427 | N | VAL | C | 18 | 35.473 | 61.129 | 10.944 | 1.00 | 53.02 | 7 |
| | ATOM | 3428 | CA | VAL | C | 18 | 34.902 | 62.398 | 10.528 | 1.00 | 53.40 | 6 |
| | ATOM | 3429 | CB | VAL | C | 18 | 34.699 | 62.421 | 9.003 | 1.00 | 53.89 | 6 |
| 25 | ATOM | 3430 | CG1 | VAL | C | 18 | 34.194 | 63.785 | 8.563 | 1.00 | 53.62 | 6 |
| | ATOM | 3431 | CG2 | VAL | C | 18 | 36.013 | 62.087 | 8.308 | 1.00 | 52.31 | 6 |
| | ATOM | 3432 | C | VAL | C | 18 | 33.589 | 62.771 | 11.201 | 1.00 | 54.75 | 6 |
| | ATOM | 3433 | O | VAL | C | 18 | 32.573 | 62.097 | 11.046 | 1.00 | 54.30 | 8 |
| | ATOM | 3434 | N | ILE | C | 19 | 33.634 | 63.870 | 11.944 | 1.00 | 56.30 | 7 |
| 30 | ATOM | 3435 | CA | ILE | C | 19 | 32.480 | 64.401 | 12.662 | 1.00 | 55.34 | 6 |
| | ATOM | 3436 | CB | ILE | C | 19 | 32.934 | 65.631 | 13.519 | 1.00 | 54.46 | 6 |
| | ATOM | 3437 | CG2 | ILE | C | 19 | 33.362 | 66.777 | 12.618 | 1.00 | 53.28 | 6 |
| | ATOM | 3438 | CG1 | ILE | C | 19 | 31.827 | 66.078 | 14.467 | 1.00 | 53.52 | 6 |
| | ATOM | 3439 | CD1 | ILE | C | 19 | 32.318 | 67.022 | 15.525 | 1.00 | 50.20 | 6 |
| 35 | ATOM | 3440 | C | ILE | C | 19 | 31.392 | 64.784 | 11.644 | 1.00 | 56.25 | 6 |
| | ATOM | 3441 | O | ILE | C | 19 | 31.675 | 65.474 | 10.653 | 1.00 | 56.64 | 8 |
| | ATOM | 3442 | N | PRO | C | 20 | 30.142 | 64.318 | 11.861 | 1.00 | 55.95 | 7 |
| | ATOM | 3443 | CD | PRO | C | 20 | 29.756 | 63.451 | 12.978 | 1.00 | 55.72 | 6 |
| | ATOM | 3444 | CA | PRO | C | 20 | 28.980 | 64.574 | 10.996 | 1.00 | 57.07 | 6 |
| 40 | ATOM | 3445 | CB | PRO | C | 20 | 27.912 | 63.627 | 11.540 | 1.00 | 55.92 | 6 |
| | ATOM | 3446 | CG | PRO | C | 20 | 28.673 | 62.639 | 12.349 | 1.00 | 57.30 | 6 |
| | ATOM | 3447 | C | PRO | C | 20 | 28.500 | 66.023 | 11.035 | 1.00 | 59.85 | 6 |
| | ATOM | 3448 | O | PRO | C | 20 | 27.326 | 66.290 | 11.270 | 1.00 | 58.63 | 8 |
| | ATOM | 3449 | N | THR | C | 21 | 29.416 | 66.947 | 10.782 | 1.00 | 64.15 | 7 |
| 45 | ATOM | 3450 | CA | THR | C | 21 | 29.123 | 68.370 | 10.797 | 1.00 | 68.52 | 6 |
| | ATOM | 3451 | CB | THR | C | 21 | 30.421 | 69.169 | 11.046 | 1.00 | 68.47 | 6 |
| | ATOM | 3452 | OG1 | THR | C | 21 | 30.496 | 69.477 | 12.440 | 1.00 | 70.47 | 8 |
| | ATOM | 3453 | CG2 | THR | C | 21 | 30.470 | 70.455 | 10.216 | 1.00 | 69.90 | 6 |
| | ATOM | 3454 | C | THR | C | 21 | 28.424 | 68.913 | 9.555 | 1.00 | 72.31 | 6 |
| 50 | ATOM | 3455 | O | THR | C | 21 | 28.826 | 68.631 | 8.412 | 1.00 | 71.25 | 8 |
| | ATOM | 3456 | N | GLN | C | 22 | 27.384 | 69.709 | 9.805 | 1.00 | 76.61 | 7 |
| | ATOM | 3457 | CA | GLN | C | 22 | 26.599 | 70.346 | 8.747 | 1.00 | 80.67 | 6 |
| | ATOM | 3458 | CB | GLN | C | 22 | 25.112 | 70.087 | 8.972 | 1.00 | 81.49 | 6 |
| | ATOM | 3459 | CG | GLN | C | 22 | 24.749 | 68.606 | 9.029 | 1.00 | 82.93 | 6 |
| 55 | ATOM | 3460 | CD | GLN | C | 22 | 23.534 | 68.351 | 9.900 | 1.00 | 83.25 | 6 |
| | ATOM | 3461 | OE1 | GLN | C | 22 | 23.566 | 68.595 | 11.120 | 1.00 | 84.14 | 8 |
| | ATOM | 3462 | NE2 | GLN | C | 22 | 22.452 | 67.867 | 9.285 | 1.00 | 83.14 | 7 |
| | ATOM | 3463 | C | GLN | C | 22 | 26.865 | 71.846 | 8.814 | 1.00 | 83.04 | 6 |
| | ATOM | 3464 | O | GLN | C | 22 | 26.382 | 72.523 | 9.730 | 1.00 | 83.36 | 8 |
| 60 | ATOM | 3465 | N | ARG | C | 23 | 27.635 | 72.357 | 7.849 | 1.00 | 85.46 | 7 |
| | ATOM | 3466 | CA | ARG | C | 23 | 27.985 | 73.783 | 7.802 | 1.00 | 86.39 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3467 | CB | ARG | C | 23 | 26.722 | 74.654 | 7.771 | 1.00 | 87.20 | 6 |
| | ATOM | 3468 | CG | ARG | C | 23 | 26.050 | 74.710 | 6.393 | 1.00 | 89.96 | 6 |
| | ATOM | 3469 | CD | ARG | C | 23 | 24.797 | 73.834 | 6.297 | 1.00 | 90.96 | 6 |
| 5 | ATOM | 3470 | NE | ARG | C | 23 | 24.282 | 73.771 | 4.920 | 1.00 | 93.30 | 7 |
| | ATOM | 3471 | CZ | ARG | C | 23 | 23.996 | 74.830 | 4.145 | 1.00 | 94.77 | 6 |
| | ATOM | 3472 | NH1 | ARG | C | 23 | 24.167 | 76.083 | 4.591 | 1.00 | 94.25 | 7 |
| | ATOM | 3473 | NH2 | ARG | C | 23 | 23.537 | 74.640 | 2.905 | 1.00 | 94.32 | 7 |
| | ATOM | 3474 | C | ARG | C | 23 | 28.828 | 74.134 | 9.013 | 1.00 | 85.61 | 6 |
| 10 | ATOM | 3475 | O | ARG | C | 23 | 29.599 | 73.302 | 9.495 | 1.00 | 85.98 | 8 |
| | ATOM | 3476 | N | ASP | C | 24 | 28.700 | 75.358 | 9.503 | 1.00 | 85.83 | 7 |
| | ATOM | 3477 | CA | ASP | C | 24 | 29.462 | 75.755 | 10.685 | 1.00 | 86.66 | 6 |
| | ATOM | 3478 | CB | ASP | C | 24 | 29.625 | 77.283 | 10.785 | 1.00 | 90.61 | 6 |
| | ATOM | 3479 | CG | ASP | C | 24 | 29.385 | 78.002 | 9.458 | 1.00 | 92.74 | 6 |
| | ATOM | 3480 | OD1 | ASP | C | 24 | 30.108 | 77.704 | 8.471 | 1.00 | 93.41 | 8 |
| 15 | ATOM | 3481 | OD2 | ASP | C | 24 | 28.468 | 78.868 | 9.418 | 1.00 | 93.68 | 8 |
| | ATOM | 3482 | C | ASP | C | 24 | 28.679 | 75.280 | 11.907 | 1.00 | 85.20 | 6 |
| | ATOM | 3483 | O | ASP | C | 24 | 29.053 | 75.591 | 13.052 | 1.00 | 85.29 | 8 |
| | ATOM | 3484 | N | ARG | C | 25 | 27.587 | 74.553 | 11.660 | 1.00 | 82.29 | 7 |
| 20 | ATOM | 3485 | CA | ARG | C | 25 | 26.761 | 74.039 | 12.742 | 1.00 | 79.75 | 6 |
| | ATOM | 3486 | CB | ARG | C | 25 | 25.422 | 73.522 | 12.210 | 1.00 | 82.55 | 6 |
| | ATOM | 3487 | CG | ARG | C | 25 | 24.428 | 74.588 | 11.781 | 1.00 | 86.91 | 6 |
| | ATOM | 3488 | CD | ARG | C | 25 | 23.026 | 73.964 | 11.594 | 1.00 | 91.01 | 6 |
| | ATOM | 3489 | NE | ARG | C | 25 | 22.007 | 74.963 | 11.252 | 1.00 | 94.97 | 7 |
| | ATOM | 3490 | CZ | ARG | C | 25 | 20.702 | 74.705 | 11.146 | 1.00 | 96.54 | 6 |
| 25 | ATOM | 3491 | NH1 | ARG | C | 25 | 20.253 | 73.471 | 11.356 | 1.00 | 97.65 | 7 |
| | ATOM | 3492 | NH2 | ARG | C | 25 | 19.844 | 75.679 | 10.837 | 1.00 | 96.40 | 7 |
| | ATOM | 3493 | C | ARG | C | 25 | 27.456 | 72.906 | 13.490 | 1.00 | 76.53 | 6 |
| | ATOM | 3494 | O | ARG | C | 25 | 28.004 | 71.987 | 12.876 | 1.00 | 78.25 | 8 |
| 30 | ATOM | 3495 | N | PRO | C | 26 | 27.449 | 72.963 | 14.829 | 1.00 | 72.39 | 7 |
| | ATOM | 3496 | CD | PRO | C | 26 | 27.074 | 74.126 | 15.647 | 1.00 | 71.70 | 6 |
| | ATOM | 3497 | CA | PRO | C | 26 | 28.073 | 71.935 | 15.660 | 1.00 | 68.13 | 6 |
| | ATOM | 3498 | CB | PRO | C | 26 | 28.087 | 72.574 | 17.050 | 1.00 | 69.12 | 6 |
| | ATOM | 3499 | CG | PRO | C | 26 | 28.066 | 74.039 | 16.770 | 1.00 | 69.98 | 6 |
| | ATOM | 3500 | C | PRO | C | 26 | 27.183 | 70.706 | 15.639 | 1.00 | 64.71 | 6 |
| 35 | ATOM | 3501 | O | PRO | C | 26 | 26.010 | 70.795 | 15.275 | 1.00 | 63.13 | 8 |
| | ATOM | 3502 | N | VAL | C | 27 | 27.735 | 69.560 | 16.019 | 1.00 | 61.55 | 7 |
| | ATOM | 3503 | CA | VAL | C | 27 | 26.937 | 68.349 | 16.081 | 1.00 | 57.92 | 6 |
| | ATOM | 3504 | CB | VAL | C | 27 | 27.805 | 67.073 | 15.948 | 1.00 | 56.85 | 6 |
| | ATOM | 3505 | CG1 | VAL | C | 27 | 27.038 | 65.860 | 16.439 | 1.00 | 54.71 | 6 |
| 40 | ATOM | 3506 | CG2 | VAL | C | 27 | 28.197 | 66.872 | 14.502 | 1.00 | 54.24 | 6 |
| | ATOM | 3507 | C | VAL | C | 27 | 26.301 | 68.400 | 17.452 | 1.00 | 56.84 | 6 |
| | ATOM | 3508 | O | VAL | C | 27 | 26.987 | 68.621 | 18.450 | 1.00 | 57.02 | 8 |
| | ATOM | 3509 | N | ALA | C | 28 | 24.989 | 68.228 | 17.506 | 1.00 | 56.11 | 7 |
| | ATOM | 3510 | CA | ALA | C | 28 | 24.302 | 68.262 | 18.783 | 1.00 | 54.82 | 6 |
| 45 | ATOM | 3511 | CB | ALA | C | 28 | 22.896 | 68.775 | 18.600 | 1.00 | 55.72 | 6 |
| | ATOM | 3512 | C | ALA | C | 28 | 24.282 | 66.879 | 19.424 | 1.00 | 54.45 | 6 |
| | ATOM | 3513 | O | ALA | C | 28 | 23.579 | 65.972 | 18.964 | 1.00 | 54.53 | 8 |
| | ATOM | 3514 | N | VAL | C | 29 | 25.067 | 66.742 | 20.488 | 1.00 | 53.25 | 7 |
| | ATOM | 3515 | CA | VAL | C | 29 | 25.191 | 65.503 | 21.235 | 1.00 | 51.65 | 6 |
| 50 | ATOM | 3516 | CB | VAL | C | 29 | 26.676 | 65.113 | 21.450 | 1.00 | 50.25 | 6 |
| | ATOM | 3517 | CG1 | VAL | C | 29 | 26.770 | 63.846 | 22.297 | 1.00 | 47.03 | 6 |
| | ATOM | 3518 | CG2 | VAL | C | 29 | 27.358 | 64.921 | 20.108 | 1.00 | 50.21 | 6 |
| | ATOM | 3519 | C | VAL | C | 29 | 24.549 | 65.670 | 22.595 | 1.00 | 52.02 | 6 |
| | ATOM | 3520 | O | VAL | C | 29 | 24.833 | 66.615 | 23.320 | 1.00 | 51.40 | 8 |
| 55 | ATOM | 3521 | N | SER | C | 30 | 23.669 | 64.745 | 22.932 | 1.00 | 53.81 | 7 |
| | ATOM | 3522 | CA | SER | C | 30 | 23.012 | 64.785 | 24.214 | 1.00 | 55.39 | 6 |
| | ATOM | 3523 | CB | SER | C | 30 | 21.495 | 64.666 | 24.034 | 1.00 | 54.53 | 6 |
| | ATOM | 3524 | OG | SER | C | 30 | 21.159 | 63.462 | 23.373 | 1.00 | 56.88 | 8 |
| | ATOM | 3525 | C | SER | C | 30 | 23.566 | 63.614 | 25.013 | 1.00 | 55.69 | 6 |
| 60 | ATOM | 3526 | O | SER | C | 30 | 23.688 | 62.504 | 24.503 | 1.00 | 56.19 | 8 |
| | ATOM | 3527 | N | VAL | C | 31 | 23.916 | 63.888 | 26.261 | 1.00 | 56.76 | 7 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3528 | CA | VAL | C | 31 | 24.466 | 62.893 | 27.174 | 1.00 | 57.06 | 6 |
| | ATOM | 3529 | CB | VAL | C | 31 | 25.871 | 63.301 | 27.640 | 1.00 | 57.34 | 6 |
| | ATOM | 3530 | CG1 | VAL | C | 31 | 26.543 | 62.141 | 28.354 | 1.00 | 57.65 | 6 |
| | ATOM | 3531 | CG2 | VAL | C | 31 | 26.674 | 63.784 | 26.467 | 1.00 | 58.89 | 6 |
| | ATOM | 3532 | C | VAL | C | 31 | 23.585 | 62.791 | 28.415 | 1.00 | 57.25 | 6 |
| 10 | ATOM | 3533 | O | VAL | C | 31 | 23.152 | 63.806 | 28.979 | 1.00 | 57.25 | 8 |
| | ATOM | 3534 | N | SER | C | 32 | 23.339 | 61.569 | 28.855 | 1.00 | 56.49 | 7 |
| | ATOM | 3535 | CA | SER | C | 32 | 22.505 | 61.356 | 30.024 | 1.00 | 57.63 | 6 |
| | ATOM | 3536 | CB | SER | C | 32 | 21.045 | 61.182 | 29.589 | 1.00 | 59.80 | 6 |
| | ATOM | 3537 | OG | SER | C | 32 | 20.220 | 60.763 | 30.667 | 1.00 | 63.17 | 8 |
| 15 | ATOM | 3538 | C | SER | C | 32 | 22.958 | 60.123 | 30.781 | 1.00 | 57.81 | 6 |
| | ATOM | 3539 | O | SER | C | 32 | 22.860 | 58.998 | 30.271 | 1.00 | 60.21 | 8 |
| | ATOM | 3540 | N | LEU | C | 33 | 23.448 | 60.317 | 31.997 | 1.00 | 56.08 | 7 |
| | ATOM | 3541 | CA | LEU | C | 33 | 23.895 | 59.182 | 32.801 | 1.00 | 55.73 | 6 |
| | ATOM | 3542 | CB | LEU | C | 33 | 25.021 | 59.581 | 33.752 | 1.00 | 53.14 | 6 |
| 20 | ATOM | 3543 | CG | LEU | C | 33 | 26.240 | 60.219 | 33.105 | 1.00 | 52.98 | 6 |
| | ATOM | 3544 | CD1 | LEU | C | 33 | 27.353 | 60.346 | 34.127 | 1.00 | 51.17 | 6 |
| | ATOM | 3545 | CD2 | LEU | C | 33 | 26.680 | 59.374 | 31.933 | 1.00 | 53.34 | 6 |
| | ATOM | 3546 | C | LEU | C | 33 | 22.752 | 58.629 | 33.624 | 1.00 | 56.29 | 6 |
| | ATOM | 3547 | O | LEU | C | 33 | 21.976 | 59.392 | 34.193 | 1.00 | 57.63 | 8 |
| 25 | ATOM | 3548 | N | LYS | C | 34 | 22.642 | 57.303 | 33.664 | 1.00 | 54.96 | 7 |
| | ATOM | 3549 | CA | LYS | C | 34 | 21.616 | 56.643 | 34.447 | 1.00 | 55.26 | 6 |
| | ATOM | 3550 | CB | LYS | C | 34 | 20.710 | 55.790 | 33.563 | 1.00 | 58.99 | 6 |
| | ATOM | 3551 | CG | LYS | C | 34 | 20.053 | 56.544 | 32.414 | 1.00 | 63.56 | 6 |
| | ATOM | 3552 | CD | LYS | C | 34 | 19.098 | 57.649 | 32.897 | 1.00 | 68.99 | 6 |
| 30 | ATOM | 3553 | CE | LYS | C | 34 | 18.499 | 58.434 | 31.705 | 1.00 | 71.13 | 6 |
| | ATOM | 3554 | NZ | LYS | C | 34 | 17.528 | 59.497 | 32.120 | 1.00 | 71.58 | 7 |
| | ATOM | 3555 | C | LYS | C | 34 | 22.410 | 55.756 | 35.369 | 1.00 | 53.96 | 6 |
| | ATOM | 3556 | O | LYS | C | 34 | 23.034 | 54.806 | 34.922 | 1.00 | 54.63 | 8 |
| | ATOM | 3557 | N | PHE | C | 35 | 22.410 | 56.064 | 36.657 | 1.00 | 53.24 | 7 |
| 35 | ATOM | 3558 | CA | PHE | C | 35 | 23.190 | 55.260 | 37.579 | 1.00 | 51.26 | 6 |
| | ATOM | 3559 | CB | PHE | C | 35 | 23.427 | 56.032 | 38.864 | 1.00 | 49.55 | 6 |
| | ATOM | 3560 | CG | PHE | C | 35 | 24.291 | 57.226 | 38.662 | 1.00 | 48.89 | 6 |
| | ATOM | 3561 | CD1 | PHE | C | 35 | 23.745 | 58.428 | 38.239 | 1.00 | 48.34 | 6 |
| | ATOM | 3562 | CD2 | PHE | C | 35 | 25.669 | 57.133 | 38.814 | 1.00 | 50.53 | 6 |
| 40 | ATOM | 3563 | CE1 | PHE | C | 35 | 24.553 | 59.526 | 37.967 | 1.00 | 47.39 | 6 |
| | ATOM | 3564 | CE2 | PHE | C | 35 | 26.488 | 58.228 | 38.542 | 1.00 | 50.75 | 6 |
| | ATOM | 3565 | CZ | PHE | C | 35 | 25.925 | 59.424 | 38.118 | 1.00 | 49.19 | 6 |
| | ATOM | 3566 | C | PHE | C | 35 | 22.608 | 53.899 | 37.849 | 1.00 | 50.23 | 6 |
| | ATOM | 3567 | O | PHE | C | 35 | 21.418 | 53.754 | 38.078 | 1.00 | 50.29 | 8 |
| 45 | ATOM | 3568 | N | ILE | C | 36 | 23.478 | 52.901 | 37.795 | 1.00 | 49.55 | 7 |
| | ATOM | 3569 | CA | ILE | C | 36 | 23.095 | 51.519 | 37.997 | 1.00 | 47.28 | 6 |
| | ATOM | 3570 | CB | ILE | C | 36 | 23.658 | 50.632 | 36.883 | 1.00 | 46.86 | 6 |
| | ATOM | 3571 | CG2 | ILE | C | 36 | 23.173 | 49.223 | 37.055 | 1.00 | 44.45 | 6 |
| | ATOM | 3572 | CG1 | ILE | C | 36 | 23.252 | 51.192 | 35.521 | 1.00 | 46.79 | 6 |
| 50 | ATOM | 3573 | CD1 | ILE | C | 36 | 21.754 | 51.310 | 35.328 | 1.00 | 48.67 | 6 |
| | ATOM | 3574 | C | ILE | C | 36 | 23.619 | 50.999 | 39.308 | 1.00 | 46.88 | 6 |
| | ATOM | 3575 | O | ILE | C | 36 | 23.052 | 50.074 | 39.866 | 1.00 | 48.98 | 8 |
| | ATOM | 3576 | N | ASN | C | 37 | 24.711 | 51.578 | 39.799 | 1.00 | 45.50 | 7 |
| | ATOM | 3577 | CA | ASN | C | 37 | 25.271 | 51.124 | 41.061 | 1.00 | 44.80 | 6 |
| 55 | ATOM | 3578 | CB | ASN | C | 37 | 25.738 | 49.678 | 40.919 | 1.00 | 44.35 | 6 |
| | ATOM | 3579 | CG | ASN | C | 37 | 25.685 | 48.919 | 42.226 | 1.00 | 47.95 | 6 |
| | ATOM | 3580 | OD1 | ASN | C | 37 | 26.077 | 49.424 | 43.285 | 1.00 | 47.36 | 8 |
| | ATOM | 3581 | ND2 | ASN | C | 37 | 25.209 | 47.688 | 42.157 | 1.00 | 50.05 | 7 |
| | ATOM | 3582 | C | ASN | C | 37 | 26.430 | 51.985 | 41.573 | 1.00 | 44.84 | 6 |
| 60 | ATOM | 3583 | O | ASN | C | 37 | 27.089 | 52.678 | 40.810 | 1.00 | 42.36 | 8 |
| | ATOM | 3584 | N | ILE | C | 38 | 26.654 | 51.939 | 42.882 | 1.00 | 45.30 | 7 |
| | ATOM | 3585 | CA | ILE | C | 38 | 27.735 | 52.671 | 43.518 | 1.00 | 46.27 | 6 |
| | ATOM | 3586 | CB | ILE | C | 38 | 27.186 | 53.759 | 44.434 | 1.00 | 44.46 | 6 |
| | ATOM | 3587 | CG2 | ILE | C | 38 | 28.319 | 54.433 | 45.178 | 1.00 | 42.73 | 6 |
| | ATOM | 3588 | CG1 | ILE | C | 38 | 26.418 | 54.770 | 43.584 | 1.00 | 42.70 | 6 |

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|----|------|------|-----|-----|---|------|--------|--------|--------|--------------|
| 5 | ATOM | 3589 | CD1 | ILE | C | 38 | 25.630 | 55.758 | 44.343 | 1.00 40.81 6 |
| | ATOM | 3590 | C | ILE | C | 38 | 28.432 | 51.585 | 44.306 | 1.00 49.67 6 |
| | ATOM | 3591 | O | ILE | C | 38 | 27.890 | 51.083 | 45.281 | 1.00 53.17 8 |
| | ATOM | 3592 | N | LEU | C | 39 | 29.636 | 51.228 | 43.872 | 1.00 51.33 7 |
| | ATOM | 3593 | CA | LEU | C | 39 | 30.378 | 50.125 | 44.468 | 1.00 53.07 6 |
| 10 | ATOM | 3594 | CB | LEU | C | 39 | 31.113 | 49.384 | 43.353 | 1.00 53.88 6 |
| | ATOM | 3595 | CG | LEU | C | 39 | 30.167 | 49.000 | 42.215 | 1.00 55.35 6 |
| | ATOM | 3596 | CD1 | LEU | C | 39 | 30.932 | 48.308 | 41.115 | 1.00 54.78 6 |
| | ATOM | 3597 | CD2 | LEU | C | 39 | 29.053 | 48.097 | 42.760 | 1.00 54.41 6 |
| | ATOM | 3598 | C | LEU | C | 39 | 31.334 | 50.367 | 45.619 | 1.00 53.89 6 |
| 15 | ATOM | 3599 | O | LEU | C | 39 | 31.386 | 49.567 | 46.558 | 1.00 53.73 8 |
| | ATOM | 3600 | N | GLU | C | 40 | 32.124 | 51.426 | 45.536 | 1.00 54.34 7 |
| | ATOM | 3601 | CA | GLU | C | 40 | 33.058 | 51.714 | 46.602 | 1.00 56.97 6 |
| | ATOM | 3602 | CB | GLU | C | 40 | 34.446 | 51.211 | 46.271 | 1.00 59.79 6 |
| | ATOM | 3603 | CG | GLU | C | 40 | 34.555 | 49.711 | 46.147 | 1.00 67.48 6 |
| 20 | ATOM | 3604 | CD | GLU | C | 40 | 35.996 | 49.266 | 45.979 | 1.00 70.43 6 |
| | ATOM | 3605 | OE1 | GLU | C | 40 | 36.647 | 49.719 | 44.998 | 1.00 71.96 8 |
| | ATOM | 3606 | OE2 | GLU | C | 40 | 36.471 | 48.476 | 46.832 | 1.00 71.19 8 |
| | ATOM | 3607 | C | GLU | C | 40 | 33.125 | 53.192 | 46.823 | 1.00 57.35 6 |
| | ATOM | 3608 | O | GLU | C | 40 | 33.163 | 53.975 | 45.886 | 1.00 58.85 8 |
| 25 | ATOM | 3609 | N | VAL | C | 41 | 33.132 | 53.572 | 48.084 | 1.00 57.50 7 |
| | ATOM | 3610 | CA | VAL | C | 41 | 33.202 | 54.964 | 48.440 | 1.00 56.50 6 |
| | ATOM | 3611 | CB | VAL | C | 41 | 31.845 | 55.447 | 49.000 | 1.00 57.37 6 |
| | ATOM | 3612 | CG1 | VAL | C | 41 | 31.972 | 56.832 | 49.567 | 1.00 56.32 6 |
| | ATOM | 3613 | CG2 | VAL | C | 41 | 30.797 | 55.437 | 47.894 | 1.00 57.94 6 |
| 30 | ATOM | 3614 | C | VAL | C | 41 | 34.289 | 55.098 | 49.486 | 1.00 55.27 6 |
| | ATOM | 3615 | O | VAL | C | 41 | 34.502 | 54.200 | 50.300 | 1.00 54.09 8 |
| | ATOM | 3616 | N | ASN | C | 42 | 34.994 | 56.216 | 49.433 | 1.00 55.74 7 |
| | ATOM | 3617 | CA | ASN | C | 42 | 36.053 | 56.504 | 50.379 | 1.00 56.05 6 |
| | ATOM | 3618 | CB | ASN | C | 42 | 37.418 | 56.169 | 49.787 | 1.00 53.93 6 |
| 35 | ATOM | 3619 | CG | ASN | C | 42 | 38.509 | 56.155 | 50.833 | 1.00 53.86 6 |
| | ATOM | 3620 | OD1 | ASN | C | 42 | 38.622 | 57.075 | 51.634 | 1.00 54.42 8 |
| | ATOM | 3621 | ND2 | ASN | C | 42 | 39.325 | 55.110 | 50.828 | 1.00 54.04 7 |
| | ATOM | 3622 | C | ASN | C | 42 | 35.947 | 57.994 | 50.635 | 1.00 58.42 6 |
| | ATOM | 3623 | O | ASN | C | 42 | 36.322 | 58.806 | 49.786 | 1.00 58.83 8 |
| 40 | ATOM | 3624 | N | GLU | C | 43 | 35.408 | 58.348 | 51.801 | 1.00 60.55 7 |
| | ATOM | 3625 | CA | GLU | C | 43 | 35.242 | 59.744 | 52.163 | 1.00 61.17 6 |
| | ATOM | 3626 | CB | GLU | C | 43 | 34.269 | 59.874 | 53.327 | 1.00 63.37 6 |
| | ATOM | 3627 | CG | GLU | C | 43 | 33.932 | 61.318 | 53.646 | 1.00 67.39 6 |
| | ATOM | 3628 | CD | GLU | C | 43 | 32.773 | 61.463 | 54.616 | 1.00 68.69 6 |
| 45 | ATOM | 3629 | OE1 | GLU | C | 43 | 32.494 | 62.613 | 55.019 | 1.00 69.27 8 |
| | ATOM | 3630 | OE2 | GLU | C | 43 | 32.142 | 60.444 | 54.964 | 1.00 68.84 8 |
| | ATOM | 3631 | C | GLU | C | 43 | 36.571 | 60.391 | 52.524 | 1.00 60.37 6 |
| | ATOM | 3632 | O | GLU | C | 43 | 36.706 | 61.611 | 52.459 | 1.00 59.71 8 |
| | ATOM | 3633 | N | ILE | C | 44 | 37.544 | 59.567 | 52.903 | 1.00 59.67 7 |
| 50 | ATOM | 3634 | CA | ILE | C | 44 | 38.874 | 60.051 | 53.254 | 1.00 60.12 6 |
| | ATOM | 3635 | CB | ILE | C | 44 | 39.727 | 58.944 | 53.908 | 1.00 60.72 6 |
| | ATOM | 3636 | CG2 | ILE | C | 44 | 41.124 | 59.469 | 54.194 | 1.00 61.61 6 |
| | ATOM | 3637 | CG1 | ILE | C | 44 | 39.081 | 58.470 | 55.206 | 1.00 62.18 6 |
| | ATOM | 3638 | CD1 | ILE | C | 44 | 39.142 | 59.479 | 56.325 | 1.00 63.46 6 |
| 55 | ATOM | 3639 | C | ILE | C | 44 | 39.617 | 60.514 | 51.998 | 1.00 59.74 6 |
| | ATOM | 3640 | O | ILE | C | 44 | 40.255 | 61.569 | 51.988 | 1.00 60.88 8 |
| | ATOM | 3641 | N | THR | C | 45 | 39.540 | 59.710 | 50.944 | 1.00 57.16 7 |
| | ATOM | 3642 | CA | THR | C | 45 | 40.221 | 60.022 | 49.698 | 1.00 54.13 6 |
| | ATOM | 3643 | CB | THR | C | 45 | 40.819 | 58.743 | 49.056 | 1.00 52.62 6 |
| 60 | ATOM | 3644 | OG1 | THR | C | 45 | 39.776 | 57.810 | 48.773 | 1.00 52.62 8 |
| | ATOM | 3645 | CG2 | THR | C | 45 | 41.812 | 58.106 | 49.985 | 1.00 52.65 6 |
| | ATOM | 3646 | C | THR | C | 45 | 39.325 | 60.706 | 48.675 | 1.00 51.85 6 |
| | ATOM | 3647 | O | THR | C | 45 | 39.801 | 61.196 | 47.664 | 1.00 51.94 8 |
| | ATOM | 3648 | N | ASN | C | 46 | 38.029 | 60.736 | 48.933 | 1.00 51.51 7 |
| | ATOM | 3649 | CA | ASN | C | 46 | 37.106 | 61.367 | 48.002 | 1.00 52.39 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3650 | CB | ASN | C | 46 | 37.420 | 62.856 | 47.890 | 1.00 | 54.02 | 6 |
| | ATOM | 3651 | CG | ASN | C | 46 | 36.525 | 63.703 | 48.766 | 1.00 | 56.29 | 6 |
| | ATOM | 3652 | OD1 | ASN | C | 46 | 36.877 | 64.821 | 49.132 | 1.00 | 59.35 | 8 |
| | ATOM | 3653 | ND2 | ASN | C | 46 | 35.357 | 63.182 | 49.093 | 1.00 | 53.30 | 7 |
| 5 | ATOM | 3654 | C | ASN | C | 46 | 37.143 | 60.711 | 46.618 | 1.00 | 52.56 | 6 |
| | ATOM | 3655 | O | ASN | C | 46 | 37.269 | 61.376 | 45.587 | 1.00 | 51.60 | 8 |
| | ATOM | 3656 | N | GLU | C | 47 | 37.013 | 59.392 | 46.610 | 1.00 | 51.63 | 7 |
| | ATOM | 3657 | CA | GLU | C | 47 | 37.023 | 58.633 | 45.376 | 1.00 | 50.56 | 6 |
| | ATOM | 3658 | CB | GLU | C | 47 | 38.307 | 57.805 | 45.300 | 1.00 | 49.50 | 6 |
| 10 | ATOM | 3659 | CG | GLU | C | 47 | 39.566 | 58.650 | 45.210 | 1.00 | 49.79 | 6 |
| | ATOM | 3660 | CD | GLU | C | 47 | 40.823 | 57.810 | 45.227 | 1.00 | 51.38 | 6 |
| | ATOM | 3661 | OE1 | GLU | C | 47 | 40.741 | 56.621 | 44.860 | 1.00 | 52.93 | 8 |
| | ATOM | 3662 | OE2 | GLU | C | 47 | 41.892 | 58.339 | 45.595 | 1.00 | 51.30 | 8 |
| | ATOM | 3663 | C | GLU | C | 47 | 35.793 | 57.734 | 45.314 | 1.00 | 48.78 | 6 |
| 15 | ATOM | 3664 | O | GLU | C | 47 | 35.403 | 57.133 | 46.300 | 1.00 | 48.46 | 8 |
| | ATOM | 3665 | N | VAL | C | 48 | 35.178 | 57.654 | 44.147 | 1.00 | 47.95 | 7 |
| | ATOM | 3666 | CA | VAL | C | 48 | 33.998 | 56.834 | 43.993 | 1.00 | 49.71 | 6 |
| | ATOM | 3667 | CB | VAL | C | 48 | 32.768 | 57.701 | 43.736 | 1.00 | 50.43 | 6 |
| | ATOM | 3668 | CG1 | VAL | C | 48 | 31.549 | 56.834 | 43.578 | 1.00 | 53.94 | 6 |
| 20 | ATOM | 3669 | CG2 | VAL | C | 48 | 32.567 | 58.645 | 44.869 | 1.00 | 52.35 | 6 |
| | ATOM | 3670 | C | VAL | C | 48 | 34.130 | 55.838 | 42.850 | 1.00 | 49.77 | 6 |
| | ATOM | 3671 | O | VAL | C | 48 | 34.686 | 56.146 | 41.802 | 1.00 | 49.93 | 8 |
| | ATOM | 3672 | N | ASP | C | 49 | 33.615 | 54.636 | 43.068 | 1.00 | 49.86 | 7 |
| | ATOM | 3673 | CA | ASP | C | 49 | 33.646 | 53.595 | 42.061 | 1.00 | 49.59 | 6 |
| 25 | ATOM | 3674 | CB | ASP | C | 49 | 34.261 | 52.331 | 42.644 | 1.00 | 51.71 | 6 |
| | ATOM | 3675 | CG | ASP | C | 49 | 34.714 | 51.366 | 41.580 | 1.00 | 51.64 | 6 |
| | ATOM | 3676 | OD1 | ASP | C | 49 | 33.992 | 51.233 | 40.581 | 1.00 | 50.25 | 8 |
| | ATOM | 3677 | OD2 | ASP | C | 49 | 35.777 | 50.736 | 41.748 | 1.00 | 51.89 | 8 |
| | ATOM | 3678 | C | ASP | C | 49 | 32.181 | 53.382 | 41.728 | 1.00 | 49.00 | 6 |
| 30 | ATOM | 3679 | O | ASP | C | 49 | 31.437 | 52.818 | 42.524 | 1.00 | 51.14 | 8 |
| | ATOM | 3680 | N | VAL | C | 50 | 31.770 | 53.840 | 40.551 | 1.00 | 48.30 | 7 |
| | ATOM | 3681 | CA | VAL | C | 50 | 30.374 | 53.757 | 40.147 | 1.00 | 48.89 | 6 |
| | ATOM | 3682 | CB | VAL | C | 50 | 29.755 | 55.185 | 40.167 | 1.00 | 51.49 | 6 |
| | ATOM | 3683 | CG1 | VAL | C | 50 | 30.212 | 55.964 | 38.944 | 1.00 | 50.49 | 6 |
| 35 | ATOM | 3684 | CG2 | VAL | C | 50 | 28.248 | 55.120 | 40.223 | 1.00 | 53.32 | 6 |
| | ATOM | 3685 | C | VAL | C | 50 | 30.130 | 53.122 | 38.771 | 1.00 | 47.56 | 6 |
| | ATOM | 3686 | O | VAL | C | 50 | 31.012 | 53.080 | 37.928 | 1.00 | 49.11 | 8 |
| | ATOM | 3687 | N | VAL | C | 51 | 28.917 | 52.621 | 38.574 | 1.00 | 44.81 | 7 |
| | ATOM | 3688 | CA | VAL | C | 51 | 28.484 | 52.003 | 37.324 | 1.00 | 43.09 | 6 |
| 40 | ATOM | 3689 | CB | VAL | C | 51 | 28.003 | 50.542 | 37.539 | 1.00 | 41.28 | 6 |
| | ATOM | 3690 | CG1 | VAL | C | 51 | 27.355 | 50.017 | 36.267 | 1.00 | 37.45 | 6 |
| | ATOM | 3691 | CG2 | VAL | C | 51 | 29.157 | 49.659 | 37.953 | 1.00 | 36.77 | 6 |
| | ATOM | 3692 | C | VAL | C | 51 | 27.300 | 52.817 | 36.781 | 1.00 | 44.98 | 6 |
| | ATOM | 3693 | O | VAL | C | 51 | 26.385 | 53.163 | 37.522 | 1.00 | 46.72 | 8 |
| 45 | ATOM | 3694 | N | PHE | C | 52 | 27.299 | 53.113 | 35.490 | 1.00 | 44.48 | 7 |
| | ATOM | 3695 | CA | PHE | C | 52 | 26.206 | 53.883 | 34.937 | 1.00 | 45.00 | 6 |
| | ATOM | 3696 | CB | PHE | C | 52 | 26.469 | 55.352 | 35.210 | 1.00 | 44.94 | 6 |
| | ATOM | 3697 | CG | PHE | C | 52 | 27.729 | 55.857 | 34.587 | 1.00 | 44.74 | 6 |
| | ATOM | 3698 | CD1 | PHE | C | 52 | 27.735 | 56.327 | 33.278 | 1.00 | 44.14 | 6 |
| 50 | ATOM | 3699 | CD2 | PHE | C | 52 | 28.921 | 55.841 | 35.299 | 1.00 | 44.43 | 6 |
| | ATOM | 3700 | CE1 | PHE | C | 52 | 28.908 | 56.771 | 32.690 | 1.00 | 45.23 | 6 |
| | ATOM | 3701 | CE2 | PHE | C | 52 | 30.102 | 56.284 | 34.722 | 1.00 | 41.52 | 6 |
| | ATOM | 3702 | CZ | PHE | C | 52 | 30.098 | 56.751 | 33.415 | 1.00 | 42.14 | 6 |
| | ATOM | 3703 | C | PHE | C | 52 | 26.048 | 53.663 | 33.443 | 1.00 | 47.73 | 6 |
| 55 | ATOM | 3704 | O | PHE | C | 52 | 26.932 | 53.102 | 32.798 | 1.00 | 49.84 | 8 |
| | ATOM | 3705 | N | TRP | C | 53 | 24.918 | 54.099 | 32.895 | 1.00 | 46.73 | 7 |
| | ATOM | 3706 | CA | TRP | C | 53 | 24.684 | 53.985 | 31.471 | 1.00 | 47.02 | 6 |
| | ATOM | 3707 | CB | TRP | C | 53 | 23.251 | 53.595 | 31.175 | 1.00 | 46.36 | 6 |
| | ATOM | 3708 | CG | TRP | C | 53 | 22.915 | 52.221 | 31.552 | 1.00 | 48.76 | 6 |
| 60 | ATOM | 3709 | CD2 | TRP | C | 53 | 21.615 | 51.636 | 31.534 | 1.00 | 50.65 | 6 |
| | ATOM | 3710 | CE2 | TRP | C | 53 | 21.748 | 50.311 | 32.002 | 1.00 | 49.66 | 6 |

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| 5 | ATOM | 3711 | CE3 | TRP | C | 53 | 20.342 | 52.106 | 31.170 | 1.00 | 51.64 | 6 |
| | ATOM | 3712 | CD1 | TRP | C | 53 | 23.765 | 51.259 | 32.008 | 1.00 | 48.94 | 6 |
| | ATOM | 3713 | NE1 | TRP | C | 53 | 23.073 | 50.107 | 32.284 | 1.00 | 48.58 | 7 |
| | ATOM | 3714 | CZ2 | TRP | C | 53 | 20.659 | 49.448 | 32.120 | 1.00 | 50.24 | 6 |
| | ATOM | 3715 | CZ3 | TRP | C | 53 | 19.258 | 51.250 | 31.286 | 1.00 | 51.60 | 6 |
| 10 | ATOM | 3716 | CH2 | TRP | C | 53 | 19.424 | 49.935 | 31.759 | 1.00 | 52.14 | 6 |
| | ATOM | 3717 | C | TRP | C | 53 | 24.940 | 55.339 | 30.862 | 1.00 | 48.39 | 6 |
| | ATOM | 3718 | O | TRP | C | 53 | 24.234 | 56.290 | 31.156 | 1.00 | 50.70 | 8 |
| | ATOM | 3719 | N | GLN | C | 54 | 25.946 | 55.429 | 30.010 | 1.00 | 49.71 | 7 |
| | ATOM | 3720 | CA | GLN | C | 54 | 26.265 | 56.691 | 29.378 | 1.00 | 50.29 | 6 |
| 15 | ATOM | 3721 | CB | GLN | C | 54 | 27.759 | 56.749 | 29.053 | 1.00 | 50.27 | 6 |
| | ATOM | 3722 | CG | GLN | C | 54 | 28.231 | 58.111 | 28.587 | 1.00 | 54.00 | 6 |
| | ATOM | 3723 | CD | GLN | C | 54 | 29.710 | 58.344 | 28.853 | 1.00 | 55.07 | 6 |
| | ATOM | 3724 | OE1 | GLN | C | 54 | 30.172 | 58.241 | 29.988 | 1.00 | 53.42 | 8 |
| | ATOM | 3725 | NE2 | GLN | C | 54 | 30.458 | 58.667 | 27.805 | 1.00 | 57.05 | 7 |
| 20 | ATOM | 3726 | C | GLN | C | 54 | 25.415 | 56.797 | 28.125 | 1.00 | 50.70 | 6 |
| | ATOM | 3727 | O | GLN | C | 54 | 25.886 | 56.617 | 27.004 | 1.00 | 52.15 | 8 |
| | ATOM | 3728 | N | GLN | C | 55 | 24.138 | 57.069 | 28.345 | 1.00 | 51.37 | 7 |
| | ATOM | 3729 | CA | GLN | C | 55 | 23.169 | 57.205 | 27.272 | 1.00 | 54.41 | 6 |
| | ATOM | 3730 | CB | GLN | C | 55 | 21.786 | 57.326 | 27.897 | 1.00 | 57.18 | 6 |
| 25 | ATOM | 3731 | CG | GLN | C | 55 | 20.667 | 57.648 | 26.948 | 1.00 | 64.94 | 6 |
| | ATOM | 3732 | CD | GLN | C | 55 | 19.313 | 57.472 | 27.617 | 1.00 | 70.65 | 6 |
| | ATOM | 3733 | OE1 | GLN | C | 55 | 19.154 | 57.760 | 28.817 | 1.00 | 73.87 | 8 |
| | ATOM | 3734 | NE2 | GLN | C | 55 | 18.325 | 56.997 | 26.849 | 1.00 | 72.08 | 7 |
| | ATOM | 3735 | C | GLN | C | 55 | 23.509 | 58.419 | 26.396 | 1.00 | 53.13 | 6 |
| 30 | ATOM | 3736 | O | GLN | C | 55 | 23.296 | 59.569 | 26.779 | 1.00 | 54.85 | 8 |
| | ATOM | 3737 | N | THR | C | 56 | 24.044 | 58.148 | 25.211 | 1.00 | 50.27 | 7 |
| | ATOM | 3738 | CA | THR | C | 56 | 24.455 | 59.193 | 24.290 | 1.00 | 48.20 | 6 |
| | ATOM | 3739 | CB | THR | C | 56 | 25.916 | 59.019 | 23.905 | 1.00 | 47.97 | 6 |
| | ATOM | 3740 | OG1 | THR | C | 56 | 26.693 | 58.795 | 25.085 | 1.00 | 51.04 | 8 |
| 35 | ATOM | 3741 | CG2 | THR | C | 56 | 26.431 | 60.243 | 23.219 | 1.00 | 46.01 | 6 |
| | ATOM | 3742 | C | THR | C | 56 | 23.633 | 59.162 | 23.023 | 1.00 | 49.71 | 6 |
| | ATOM | 3743 | O | THR | C | 56 | 23.216 | 58.095 | 22.568 | 1.00 | 49.78 | 8 |
| | ATOM | 3744 | N | THR | C | 57 | 23.393 | 60.340 | 22.454 | 1.00 | 49.24 | 7 |
| | ATOM | 3745 | CA | THR | C | 57 | 22.619 | 60.436 | 21.221 | 1.00 | 49.62 | 6 |
| 40 | ATOM | 3746 | CB | THR | C | 57 | 21.122 | 60.592 | 21.501 | 1.00 | 49.45 | 6 |
| | ATOM | 3747 | OG1 | THR | C | 57 | 20.640 | 59.440 | 22.206 | 1.00 | 49.55 | 8 |
| | ATOM | 3748 | CG2 | THR | C | 57 | 20.368 | 60.722 | 20.191 | 1.00 | 51.01 | 6 |
| | ATOM | 3749 | C | THR | C | 57 | 23.057 | 61.608 | 20.368 | 1.00 | 48.68 | 6 |
| | ATOM | 3750 | O | THR | C | 57 | 23.423 | 62.649 | 20.888 | 1.00 | 51.05 | 8 |
| 45 | ATOM | 3751 | N | TRP | C | 58 | 23.033 | 61.428 | 19.056 | 1.00 | 45.80 | 7 |
| | ATOM | 3752 | CA | TRP | C | 58 | 23.415 | 62.487 | 18.145 | 1.00 | 45.33 | 6 |
| | ATOM | 3753 | CB | TRP | C | 58 | 24.934 | 62.702 | 18.146 | 1.00 | 44.23 | 6 |
| | ATOM | 3754 | CG | TRP | C | 58 | 25.733 | 61.584 | 17.556 | 1.00 | 45.68 | 6 |
| | ATOM | 3755 | CD2 | TRP | C | 58 | 26.221 | 60.428 | 18.241 | 1.00 | 43.51 | 6 |
| 50 | ATOM | 3756 | CE2 | TRP | C | 58 | 26.896 | 59.642 | 17.296 | 1.00 | 41.95 | 6 |
| | ATOM | 3757 | CE3 | TRP | C | 58 | 26.150 | 59.983 | 19.566 | 1.00 | 44.75 | 6 |
| | ATOM | 3758 | CD1 | TRP | C | 58 | 26.120 | 61.453 | 16.264 | 1.00 | 41.99 | 6 |
| | ATOM | 3759 | NE1 | TRP | C | 58 | 26.818 | 60.292 | 16.097 | 1.00 | 43.07 | 7 |
| | ATOM | 3760 | CZ2 | TRP | C | 58 | 27.498 | 58.436 | 17.625 | 1.00 | 42.44 | 6 |
| 55 | ATOM | 3761 | CZ3 | TRP | C | 58 | 26.748 | 58.778 | 19.894 | 1.00 | 45.66 | 6 |
| | ATOM | 3762 | CH2 | TRP | C | 58 | 27.414 | 58.020 | 18.926 | 1.00 | 44.08 | 6 |
| | ATOM | 3763 | C | TRP | C | 58 | 22.915 | 62.107 | 16.772 | 1.00 | 46.80 | 6 |
| | ATOM | 3764 | O | TRP | C | 58 | 22.315 | 61.054 | 16.603 | 1.00 | 45.26 | 8 |
| | ATOM | 3765 | N | SER | C | 59 | 23.157 | 62.959 | 15.788 | 1.00 | 50.21 | 7 |
| 60 | ATOM | 3766 | CA | SER | C | 59 | 22.663 | 62.684 | 14.452 | 1.00 | 53.47 | 6 |
| | ATOM | 3767 | CB | SER | C | 59 | 21.536 | 63.657 | 14.128 | 1.00 | 54.42 | 6 |
| | ATOM | 3768 | OG | SER | C | 59 | 20.707 | 63.146 | 13.104 | 1.00 | 59.88 | 8 |
| | ATOM | 3769 | C | SER | C | 59 | 23.733 | 62.752 | 13.376 | 1.00 | 54.85 | 6 |
| | ATOM | 3770 | O | SER | C | 59 | 24.541 | 63.682 | 13.343 | 1.00 | 54.12 | 8 |
| | ATOM | 3771 | N | ASP | C | 60 | 23.727 | 61.745 | 12.503 | 1.00 | 57.21 | 7 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3772 | CA | ASP | C | 60 | 24.677 | 61.646 | 11.396 | 1.00 | 59.27 | 6 |
| | ATOM | 3773 | CB | ASP | C | 60 | 25.680 | 60.517 | 11.650 | 1.00 | 59.62 | 6 |
| | ATOM | 3774 | CG | ASP | C | 60 | 26.786 | 60.472 | 10.615 | 1.00 | 61.35 | 6 |
| 5 | ATOM | 3775 | OD1 | ASP | C | 60 | 26.553 | 60.894 | 9.462 | 1.00 | 60.03 | 8 |
| | ATOM | 3776 | OD2 | ASP | C | 60 | 27.890 | 59.996 | 10.957 | 1.00 | 62.69 | 8 |
| | ATOM | 3777 | C | ASP | C | 60 | 23.842 | 61.317 | 10.172 | 1.00 | 61.10 | 6 |
| | ATOM | 3778 | O | ASP | C | 60 | 23.493 | 60.163 | 9.940 | 1.00 | 61.72 | 8 |
| | ATOM | 3779 | N | ARG | C | 61 | 23.509 | 62.338 | 9.396 | 1.00 | 63.66 | 7 |
| 10 | ATOM | 3780 | CA | ARG | C | 61 | 22.689 | 62.153 | 8.201 | 1.00 | 65.73 | 6 |
| | ATOM | 3781 | CB | ARG | C | 61 | 22.276 | 63.516 | 7.628 | 1.00 | 68.89 | 6 |
| | ATOM | 3782 | CG | ARG | C | 61 | 21.106 | 64.221 | 8.348 | 1.00 | 74.08 | 6 |
| | ATOM | 3783 | CD | ARG | C | 61 | 20.624 | 65.417 | 7.517 | 1.00 | 79.55 | 6 |
| | ATOM | 3784 | NE | ARG | C | 61 | 19.438 | 66.085 | 8.059 | 1.00 | 84.63 | 7 |
| | ATOM | 3785 | CZ | ARG | C | 61 | 18.810 | 67.101 | 7.457 | 1.00 | 87.07 | 6 |
| 15 | ATOM | 3786 | NH1 | ARG | C | 61 | 19.257 | 67.572 | 6.291 | 1.00 | 88.09 | 7 |
| | ATOM | 3787 | NH2 | ARG | C | 61 | 17.721 | 67.636 | 8.005 | 1.00 | 87.40 | 7 |
| | ATOM | 3788 | C | ARG | C | 61 | 23.322 | 61.310 | 7.083 | 1.00 | 64.92 | 6 |
| | ATOM | 3789 | O | ARG | C | 61 | 22.604 | 60.783 | 6.225 | 1.00 | 65.71 | 8 |
| 20 | ATOM | 3790 | N | THR | C | 62 | 24.648 | 61.176 | 7.078 | 1.00 | 62.18 | 7 |
| | ATOM | 3791 | CA | THR | C | 62 | 25.301 | 60.393 | 6.038 | 1.00 | 60.64 | 6 |
| | ATOM | 3792 | CB | THR | C | 62 | 26.840 | 60.568 | 6.056 | 1.00 | 61.65 | 6 |
| | ATOM | 3793 | OG1 | THR | C | 62 | 27.389 | 59.999 | 7.256 | 1.00 | 63.35 | 8 |
| | ATOM | 3794 | CG2 | THR | C | 62 | 27.207 | 62.045 | 5.983 | 1.00 | 61.52 | 6 |
| 25 | ATOM | 3795 | C | THR | C | 62 | 24.970 | 58.917 | 6.211 | 1.00 | 60.11 | 6 |
| | ATOM | 3796 | O | THR | C | 62 | 25.303 | 58.095 | 5.354 | 1.00 | 61.77 | 8 |
| | ATOM | 3797 | N | LEU | C | 63 | 24.313 | 58.592 | 7.321 | 1.00 | 58.17 | 7 |
| | ATOM | 3798 | CA | LEU | C | 63 | 23.919 | 57.219 | 7.621 | 1.00 | 57.53 | 6 |
| | ATOM | 3799 | CB | LEU | C | 63 | 24.079 | 56.929 | 9.111 | 1.00 | 54.69 | 6 |
| 30 | ATOM | 3800 | CG | LEU | C | 63 | 25.442 | 57.142 | 9.750 | 1.00 | 55.50 | 6 |
| | ATOM | 3801 | CD1 | LEU | C | 63 | 25.327 | 56.938 | 11.263 | 1.00 | 54.27 | 6 |
| | ATOM | 3802 | CD2 | LEU | C | 63 | 26.449 | 56.178 | 9.139 | 1.00 | 55.93 | 6 |
| | ATOM | 3803 | C | LEU | C | 63 | 22.455 | 56.977 | 7.242 | 1.00 | 58.42 | 6 |
| | ATOM | 3804 | O | LEU | C | 63 | 22.010 | 55.830 | 7.147 | 1.00 | 58.94 | 8 |
| 35 | ATOM | 3805 | N | ALA | C | 64 | 21.707 | 58.055 | 7.037 | 1.00 | 58.80 | 7 |
| | ATOM | 3806 | CA | ALA | C | 64 | 20.291 | 57.928 | 6.703 | 1.00 | 61.86 | 6 |
| | ATOM | 3807 | CB | ALA | C | 64 | 19.666 | 59.310 | 6.522 | 1.00 | 61.89 | 6 |
| | ATOM | 3808 | C | ALA | C | 64 | 20.081 | 57.087 | 5.450 | 1.00 | 63.09 | 6 |
| | ATOM | 3809 | O | ALA | C | 64 | 20.840 | 57.179 | 4.481 | 1.00 | 63.27 | 8 |
| 40 | ATOM | 3810 | N | TRP | C | 65 | 19.055 | 56.249 | 5.485 | 1.00 | 65.02 | 7 |
| | ATOM | 3811 | CA | TRP | C | 65 | 18.749 | 55.381 | 4.355 | 1.00 | 66.31 | 6 |
| | ATOM | 3812 | CB | TRP | C | 65 | 19.329 | 53.989 | 4.600 | 1.00 | 64.14 | 6 |
| | ATOM | 3813 | CG | TRP | C | 65 | 18.597 | 53.208 | 5.687 | 1.00 | 62.22 | 6 |
| | ATOM | 3814 | CD2 | TRP | C | 65 | 18.962 | 53.110 | 7.074 | 1.00 | 57.97 | 6 |
| 45 | ATOM | 3815 | CE2 | TRP | C | 65 | 18.025 | 52.247 | 7.694 | 1.00 | 56.42 | 6 |
| | ATOM | 3816 | CE3 | TRP | C | 65 | 19.985 | 53.666 | 7.848 | 1.00 | 55.52 | 6 |
| | ATOM | 3817 | CD1 | TRP | C | 65 | 17.475 | 52.430 | 5.533 | 1.00 | 60.23 | 6 |
| | ATOM | 3818 | NE1 | TRP | C | 65 | 17.131 | 51.849 | 6.734 | 1.00 | 57.79 | 7 |
| | ATOM | 3819 | CZ2 | TRP | C | 65 | 18.088 | 51.926 | 9.049 | 1.00 | 55.30 | 6 |
| 50 | ATOM | 3820 | CZ3 | TRP | C | 65 | 20.047 | 53.350 | 9.195 | 1.00 | 56.61 | 6 |
| | ATOM | 3821 | CH2 | TRP | C | 65 | 19.102 | 52.484 | 9.784 | 1.00 | 56.47 | 6 |
| | ATOM | 3822 | C | TRP | C | 65 | 17.238 | 55.287 | 4.252 | 1.00 | 68.58 | 6 |
| | ATOM | 3823 | O | TRP | C | 65 | 16.540 | 55.365 | 5.268 | 1.00 | 67.72 | 8 |
| | ATOM | 3824 | N | ASN | C | 66 | 16.728 | 55.113 | 3.037 | 1.00 | 72.17 | 7 |
| 55 | ATOM | 3825 | CA | ASN | C | 66 | 15.283 | 55.011 | 2.882 | 1.00 | 75.21 | 6 |
| | ATOM | 3826 | CB | ASN | C | 66 | 14.863 | 55.013 | 1.408 | 1.00 | 77.34 | 6 |
| | ATOM | 3827 | CG | ASN | C | 66 | 13.355 | 55.190 | 1.244 | 1.00 | 79.16 | 6 |
| | ATOM | 3828 | OD1 | ASN | C | 66 | 12.845 | 55.261 | 0.119 | 1.00 | 80.81 | 8 |
| | ATOM | 3829 | ND2 | ASN | C | 66 | 12.633 | 55.267 | 2.374 | 1.00 | 77.07 | 7 |
| | ATOM | 3830 | C | ASN | C | 66 | 14.802 | 53.730 | 3.532 | 1.00 | 74.77 | 6 |
| 60 | ATOM | 3831 | O | ASN | C | 66 | 15.431 | 52.675 | 3.383 | 1.00 | 75.31 | 8 |
| | ATOM | 3832 | N | SER | C | 67 | 13.685 | 53.816 | 4.244 | 1.00 | 73.52 | 7 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3833 | CA | SER | C | 67 | 13.166 | 52.647 | 4.920 | 1.00 | 73.52 | 6 |
| | ATOM | 3834 | CB | SER | C | 67 | 13.451 | 52.759 | 6.411 | 1.00 | 72.63 | 6 |
| | ATOM | 3835 | OG | SER | C | 67 | 12.985 | 53.994 | 6.914 | 1.00 | 70.04 | 8 |
| 5 | ATOM | 3836 | C | SER | C | 67 | 11.684 | 52.469 | 4.702 | 1.00 | 75.29 | 6 |
| | ATOM | 3837 | O | SER | C | 67 | 11.010 | 51.788 | 5.493 | 1.00 | 75.31 | 8 |
| | ATOM | 3838 | N | SER | C | 68 | 11.165 | 53.077 | 3.639 | 1.00 | 77.57 | 7 |
| | ATOM | 3839 | CA | SER | C | 68 | 9.739 | 52.957 | 3.356 | 1.00 | 78.39 | 6 |
| | ATOM | 3840 | CB | SER | C | 68 | 9.327 | 53.874 | 2.187 | 1.00 | 77.79 | 6 |
| 10 | ATOM | 3841 | OG | SER | C | 68 | 10.010 | 53.570 | 0.983 | 1.00 | 77.16 | 8 |
| | ATOM | 3842 | C | SER | C | 68 | 9.398 | 51.498 | 3.051 | 1.00 | 78.91 | 6 |
| | ATOM | 3843 | O | SER | C | 68 | 8.242 | 51.165 | 2.802 | 1.00 | 78.88 | 8 |
| | ATOM | 3844 | N | HIS | C | 69 | 10.415 | 50.634 | 3.090 | 1.00 | 80.17 | 7 |
| | ATOM | 3845 | CA | HIS | C | 69 | 10.252 | 49.197 | 2.824 | 1.00 | 81.55 | 6 |
| | ATOM | 3846 | CB | HIS | C | 69 | 10.307 | 48.935 | 1.319 | 1.00 | 84.67 | 6 |
| 15 | ATOM | 3847 | CG | HIS | C | 69 | 9.327 | 49.755 | 0.542 | 1.00 | 88.75 | 6 |
| | ATOM | 3848 | CD2 | HIS | C | 69 | 8.119 | 49.436 | 0.014 | 1.00 | 89.38 | 6 |
| | ATOM | 3849 | ND1 | HIS | C | 69 | 9.479 | 51.115 | 0.359 | 1.00 | 89.98 | 7 |
| | ATOM | 3850 | CE1 | HIS | C | 69 | 8.405 | 51.600 | -0.239 | 1.00 | 91.29 | 6 |
| 20 | ATOM | 3851 | NE2 | HIS | C | 69 | 7.564 | 50.602 | -0.458 | 1.00 | 91.72 | 7 |
| | ATOM | 3852 | C | HIS | C | 69 | 11.363 | 48.406 | 3.514 | 1.00 | 80.62 | 6 |
| | ATOM | 3853 | O | HIS | C | 69 | 11.740 | 47.318 | 3.072 | 1.00 | 79.15 | 8 |
| | ATOM | 3854 | N | SER | C | 70 | 11.867 | 48.961 | 4.614 | 1.00 | 79.62 | 7 |
| | ATOM | 3855 | CA | SER | C | 70 | 12.950 | 48.341 | 5.355 | 1.00 | 77.30 | 6 |
| 25 | ATOM | 3856 | CB | SER | C | 70 | 14.262 | 48.818 | 4.739 | 1.00 | 77.47 | 6 |
| | ATOM | 3857 | OG | SER | C | 70 | 14.107 | 48.991 | 3.336 | 1.00 | 74.00 | 8 |
| | ATOM | 3858 | C | SER | C | 70 | 12.880 | 48.746 | 6.836 | 1.00 | 76.56 | 6 |
| | ATOM | 3859 | O | SER | C | 70 | 12.168 | 49.686 | 7.193 | 1.00 | 77.11 | 8 |
| | ATOM | 3860 | N | PRO | C | 71 | 13.587 | 48.014 | 7.726 | 1.00 | 76.29 | 7 |
| 30 | ATOM | 3861 | CD | PRO | C | 71 | 14.305 | 46.733 | 7.544 | 1.00 | 75.52 | 6 |
| | ATOM | 3862 | CA | PRO | C | 71 | 13.538 | 48.401 | 9.143 | 1.00 | 74.74 | 6 |
| | ATOM | 3863 | CB | PRO | C | 71 | 14.366 | 47.322 | 9.843 | 1.00 | 75.26 | 6 |
| | ATOM | 3864 | CG | PRO | C | 71 | 14.241 | 46.124 | 8.936 | 1.00 | 75.64 | 6 |
| | ATOM | 3865 | C | PRO | C | 71 | 14.202 | 49.771 | 9.235 | 1.00 | 73.61 | 6 |
| 35 | ATOM | 3866 | O | PRO | C | 71 | 15.042 | 50.125 | 8.401 | 1.00 | 72.22 | 8 |
| | ATOM | 3867 | N | ASP | C | 72 | 13.828 | 50.537 | 10.247 | 1.00 | 72.60 | 7 |
| | ATOM | 3868 | CA | ASP | C | 72 | 14.377 | 51.869 | 10.414 | 1.00 | 70.96 | 6 |
| | ATOM | 3869 | CB | ASP | C | 72 | 13.277 | 52.795 | 10.899 | 1.00 | 75.25 | 6 |
| | ATOM | 3870 | CG | ASP | C | 72 | 11.919 | 52.353 | 10.415 | 1.00 | 78.33 | 6 |
| 40 | ATOM | 3871 | OD1 | ASP | C | 72 | 11.633 | 52.512 | 9.199 | 1.00 | 79.88 | 8 |
| | ATOM | 3872 | OD2 | ASP | C | 72 | 11.150 | 51.821 | 11.256 | 1.00 | 79.56 | 8 |
| | ATOM | 3873 | C | ASP | C | 72 | 15.519 | 51.835 | 11.411 | 1.00 | 68.36 | 6 |
| | ATOM | 3874 | O | ASP | C | 72 | 16.046 | 52.887 | 11.799 | 1.00 | 66.88 | 8 |
| | ATOM | 3875 | N | GLN | C | 73 | 15.883 | 50.625 | 11.838 | 1.00 | 63.81 | 7 |
| 45 | ATOM | 3876 | CA | GLN | C | 73 | 17.001 | 50.485 | 12.756 | 1.00 | 61.20 | 6 |
| | ATOM | 3877 | CB | GLN | C | 73 | 16.537 | 50.494 | 14.191 | 1.00 | 61.12 | 6 |
| | ATOM | 3878 | CG | GLN | C | 73 | 16.121 | 51.802 | 14.749 | 1.00 | 62.71 | 6 |
| | ATOM | 3879 | CD | GLN | C | 73 | 15.665 | 51.603 | 16.163 | 1.00 | 64.60 | 6 |
| | ATOM | 3880 | OE1 | GLN | C | 73 | 14.784 | 50.779 | 16.421 | 1.00 | 67.49 | 8 |
| 50 | ATOM | 3881 | NE2 | GLN | C | 73 | 16.267 | 52.329 | 17.099 | 1.00 | 66.00 | 7 |
| | ATOM | 3882 | C | GLN | C | 73 | 17.842 | 49.232 | 12.583 | 1.00 | 59.70 | 6 |
| | ATOM | 3883 | O | GLN | C | 73 | 17.350 | 48.167 | 12.213 | 1.00 | 61.26 | 8 |
| | ATOM | 3884 | N | VAL | C | 74 | 19.122 | 49.369 | 12.893 | 1.00 | 56.05 | 7 |
| | ATOM | 3885 | CA | VAL | C | 74 | 20.050 | 48.260 | 12.825 | 1.00 | 52.11 | 6 |
| 55 | ATOM | 3886 | CB | VAL | C | 74 | 20.736 | 48.177 | 11.454 | 1.00 | 52.42 | 6 |
| | ATOM | 3887 | CG1 | VAL | C | 74 | 19.732 | 47.788 | 10.397 | 1.00 | 51.61 | 6 |
| | ATOM | 3888 | CG2 | VAL | C | 74 | 21.376 | 49.507 | 11.112 | 1.00 | 52.96 | 6 |
| | ATOM | 3889 | C | VAL | C | 74 | 21.095 | 48.498 | 13.891 | 1.00 | 50.29 | 6 |
| | ATOM | 3890 | O | VAL | C | 74 | 21.277 | 49.626 | 14.332 | 1.00 | 49.79 | 8 |
| 60 | ATOM | 3891 | N | SER | C | 75 | 21.754 | 47.431 | 14.323 | 1.00 | 48.56 | 7 |
| | ATOM | 3892 | CA | SER | C | 75 | 22.809 | 47.533 | 15.318 | 1.00 | 45.56 | 6 |
| | ATOM | 3893 | CB | SER | C | 75 | 22.784 | 46.337 | 16.257 | 1.00 | 43.40 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3894 | OG | SER | C | 75 | 21.818 | 46.521 | 17.269 | 1.00 | 43.99 | 8 |
| | ATOM | 3895 | C | SER | C | 75 | 24.146 | 47.611 | 14.595 | 1.00 | 44.84 | 6 |
| | ATOM | 3896 | O | SER | C | 75 | 24.519 | 46.703 | 13.858 | 1.00 | 47.60 | 8 |
| 5 | ATOM | 3897 | N | VAL | C | 76 | 24.858 | 48.712 | 14.811 | 1.00 | 43.51 | 7 |
| | ATOM | 3898 | CA | VAL | C | 76 | 26.140 | 48.941 | 14.165 | 1.00 | 42.84 | 6 |
| | ATOM | 3899 | CB | VAL | C | 76 | 26.122 | 50.273 | 13.412 | 1.00 | 41.76 | 6 |
| | ATOM | 3900 | CG1 | VAL | C | 76 | 27.441 | 50.504 | 12.741 | 1.00 | 42.71 | 6 |
| | ATOM | 3901 | CG2 | VAL | C | 76 | 25.003 | 50.279 | 12.403 | 1.00 | 40.70 | 6 |
| 10 | ATOM | 3902 | C | VAL | C | 76 | 27.294 | 48.961 | 15.153 | 1.00 | 42.64 | 6 |
| | ATOM | 3903 | O | VAL | C | 76 | 27.194 | 49.542 | 16.227 | 1.00 | 45.77 | 8 |
| | ATOM | 3904 | N | PRO | C | 77 | 28.409 | 48.313 | 14.812 | 1.00 | 41.78 | 7 |
| | ATOM | 3905 | CD | PRO | C | 77 | 28.644 | 47.345 | 13.737 | 1.00 | 41.15 | 6 |
| | ATOM | 3906 | CA | PRO | C | 77 | 29.532 | 48.326 | 15.748 | 1.00 | 41.64 | 6 |
| | ATOM | 3907 | CB | PRO | C | 77 | 30.527 | 47.370 | 15.108 | 1.00 | 40.47 | 6 |
| 15 | ATOM | 3908 | CG | PRO | C | 77 | 29.654 | 46.432 | 14.379 | 1.00 | 42.43 | 6 |
| | ATOM | 3909 | C | PRO | C | 77 | 30.074 | 49.746 | 15.860 | 1.00 | 41.29 | 6 |
| | ATOM | 3910 | O | PRO | C | 77 | 30.123 | 50.489 | 14.881 | 1.00 | 38.61 | 8 |
| | ATOM | 3911 | N | ILE | C | 78 | 30.469 | 50.111 | 17.070 | 1.00 | 41.82 | 7 |
| 20 | ATOM | 3912 | CA | ILE | C | 78 | 31.000 | 51.433 | 17.359 | 1.00 | 41.93 | 6 |
| | ATOM | 3913 | CB | ILE | C | 78 | 31.439 | 51.489 | 18.837 | 1.00 | 42.16 | 6 |
| | ATOM | 3914 | CG2 | ILE | C | 78 | 32.370 | 52.634 | 19.107 | 1.00 | 42.14 | 6 |
| | ATOM | 3915 | CG1 | ILE | C | 78 | 30.193 | 51.601 | 19.696 | 1.00 | 44.77 | 6 |
| | ATOM | 3916 | CD1 | ILE | C | 78 | 29.251 | 52.676 | 19.216 | 1.00 | 44.16 | 6 |
| 25 | ATOM | 3917 | C | ILE | C | 78 | 32.149 | 51.813 | 16.450 | 1.00 | 42.57 | 6 |
| | ATOM | 3918 | O | ILE | C | 78 | 32.287 | 52.963 | 16.063 | 1.00 | 45.18 | 8 |
| | ATOM | 3919 | N | SER | C | 79 | 32.963 | 50.829 | 16.100 | 1.00 | 43.18 | 7 |
| | ATOM | 3920 | CA | SER | C | 79 | 34.120 | 51.030 | 15.241 | 1.00 | 43.52 | 6 |
| | ATOM | 3921 | CB | SER | C | 79 | 34.969 | 49.768 | 15.242 | 1.00 | 43.74 | 6 |
| 30 | ATOM | 3922 | OG | SER | C | 79 | 34.189 | 48.637 | 14.910 | 1.00 | 43.50 | 8 |
| | ATOM | 3923 | C | SER | C | 79 | 33.810 | 51.415 | 13.804 | 1.00 | 43.41 | 6 |
| | ATOM | 3924 | O | SER | C | 79 | 34.698 | 51.838 | 13.082 | 1.00 | 44.10 | 8 |
| | ATOM | 3925 | N | SER | C | 80 | 32.562 | 51.264 | 13.380 | 1.00 | 43.62 | 7 |
| | ATOM | 3926 | CA | SER | C | 80 | 32.180 | 51.604 | 12.012 | 1.00 | 44.83 | 6 |
| | ATOM | 3927 | CB | SER | C | 80 | 31.260 | 50.534 | 11.441 | 1.00 | 44.21 | 6 |
| 35 | ATOM | 3928 | OG | SER | C | 80 | 31.915 | 49.284 | 11.380 | 1.00 | 52.55 | 8 |
| | ATOM | 3929 | C | SER | C | 80 | 31.482 | 52.956 | 11.908 | 1.00 | 46.57 | 6 |
| | ATOM | 3930 | O | SER | C | 80 | 31.050 | 53.355 | 10.829 | 1.00 | 46.16 | 8 |
| | ATOM | 3931 | N | LEU | C | 81 | 31.366 | 53.649 | 13.035 | 1.00 | 46.49 | 7 |
| 40 | ATOM | 3932 | CA | LEU | C | 81 | 30.720 | 54.952 | 13.080 | 1.00 | 45.86 | 6 |
| | ATOM | 3933 | CB | LEU | C | 81 | 29.467 | 54.891 | 13.935 | 1.00 | 45.00 | 6 |
| | ATOM | 3934 | CG | LEU | C | 81 | 28.421 | 53.827 | 13.653 | 1.00 | 46.58 | 6 |
| | ATOM | 3935 | CD1 | LEU | C | 81 | 27.488 | 53.701 | 14.839 | 1.00 | 45.04 | 6 |
| | ATOM | 3936 | CD2 | LEU | C | 81 | 27.667 | 54.198 | 12.405 | 1.00 | 47.69 | 6 |
| 45 | ATOM | 3937 | C | LEU | C | 81 | 31.645 | 55.973 | 13.718 | 1.00 | 46.18 | 6 |
| | ATOM | 3938 | O | LEU | C | 81 | 32.636 | 55.613 | 14.355 | 1.00 | 50.36 | 8 |
| | ATOM | 3939 | N | TRP | C | 82 | 31.323 | 57.249 | 13.536 | 1.00 | 43.58 | 7 |
| | ATOM | 3940 | CA | TRP | C | 82 | 32.086 | 58.303 | 14.161 | 1.00 | 39.79 | 6 |
| | ATOM | 3941 | CB | TRP | C | 82 | 31.860 | 59.639 | 13.463 | 1.00 | 41.96 | 6 |
| 50 | ATOM | 3942 | CG | TRP | C | 82 | 32.342 | 60.817 | 14.278 | 1.00 | 44.12 | 6 |
| | ATOM | 3943 | CD2 | TRP | C | 82 | 31.577 | 61.569 | 15.230 | 1.00 | 44.19 | 6 |
| | ATOM | 3944 | CE2 | TRP | C | 82 | 32.453 | 62.504 | 15.823 | 1.00 | 43.39 | 6 |
| | ATOM | 3945 | CE3 | TRP | C | 82 | 30.234 | 61.540 | 15.645 | 1.00 | 44.58 | 6 |
| | ATOM | 3946 | CD1 | TRP | C | 82 | 33.611 | 61.318 | 14.327 | 1.00 | 43.74 | 6 |
| | ATOM | 3947 | NE1 | TRP | C | 82 | 33.686 | 62.327 | 15.252 | 1.00 | 44.54 | 7 |
| 55 | ATOM | 3948 | CZ2 | TRP | C | 82 | 32.033 | 63.405 | 16.809 | 1.00 | 42.68 | 6 |
| | ATOM | 3949 | CZ3 | TRP | C | 82 | 29.818 | 62.430 | 16.623 | 1.00 | 43.22 | 6 |
| | ATOM | 3950 | CH2 | TRP | C | 82 | 30.717 | 63.352 | 17.195 | 1.00 | 43.77 | 6 |
| | ATOM | 3951 | C | TRP | C | 82 | 31.426 | 58.348 | 15.514 | 1.00 | 40.00 | 6 |
| 60 | ATOM | 3952 | O | TRP | C | 82 | 30.219 | 58.174 | 15.619 | 1.00 | 39.36 | 8 |
| | ATOM | 3953 | N | VAL | C | 83 | 32.201 | 58.574 | 16.557 | 1.00 | 40.23 | 7 |
| | ATOM | 3954 | CA | VAL | C | 83 | 31.626 | 58.649 | 17.887 | 1.00 | 39.34 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 3955 | CB | VAL | C | 83 | 31.891 | 57.325 | 18.657 | 1.00 | 38.82 | 6 |
| | ATOM | 3956 | CG1 | VAL | C | 83 | 31.587 | 57.479 | 20.109 | 1.00 | 39.50 | 6 |
| | ATOM | 3957 | CG2 | VAL | C | 83 | 31.021 | 56.219 | 18.087 | 1.00 | 38.81 | 6 |
| 5 | ATOM | 3958 | C | VAL | C | 83 | 32.205 | 59.860 | 18.624 | 1.00 | 40.30 | 6 |
| | ATOM | 3959 | O | VAL | C | 83 | 33.365 | 60.222 | 18.428 | 1.00 | 41.45 | 8 |
| | ATOM | 3960 | N | PRO | C | 84 | 31.386 | 60.528 | 19.451 | 1.00 | 38.82 | 7 |
| | ATOM | 3961 | CD | PRO | C | 84 | 29.948 | 60.288 | 19.644 | 1.00 | 40.83 | 6 |
| | ATOM | 3962 | CA | PRO | C | 84 | 31.812 | 61.698 | 20.220 | 1.00 | 36.19 | 6 |
| 10 | ATOM | 3963 | CB | PRO | C | 84 | 30.580 | 62.022 | 21.058 | 1.00 | 37.66 | 6 |
| | ATOM | 3964 | CG | PRO | C | 84 | 29.479 | 61.609 | 20.201 | 1.00 | 39.39 | 6 |
| | ATOM | 3965 | C | PRO | C | 84 | 32.999 | 61.358 | 21.098 | 1.00 | 34.25 | 6 |
| | ATOM | 3966 | O | PRO | C | 84 | 32.987 | 60.351 | 21.788 | 1.00 | 35.16 | 8 |
| | ATOM | 3967 | N | ASP | C | 85 | 34.016 | 62.206 | 21.093 | 1.00 | 33.39 | 7 |
| | ATOM | 3968 | CA | ASP | C | 85 | 35.192 | 61.949 | 21.909 | 1.00 | 34.67 | 6 |
| 15 | ATOM | 3969 | CB | ASP | C | 85 | 36.423 | 62.588 | 21.270 | 1.00 | 35.95 | 6 |
| | ATOM | 3970 | CG | ASP | C | 85 | 36.260 | 64.056 | 21.046 | 1.00 | 35.70 | 6 |
| | ATOM | 3971 | OD1 | ASP | C | 85 | 35.159 | 64.468 | 20.662 | 1.00 | 34.85 | 8 |
| | ATOM | 3972 | OD2 | ASP | C | 85 | 37.234 | 64.798 | 21.238 | 1.00 | 38.52 | 8 |
| | ATOM | 3973 | C | ASP | C | 85 | 35.005 | 62.452 | 23.326 | 1.00 | 36.34 | 6 |
| 20 | ATOM | 3974 | O | ASP | C | 85 | 35.806 | 63.229 | 23.841 | 1.00 | 39.41 | 8 |
| | ATOM | 3975 | N | LEU | C | 86 | 33.941 | 61.978 | 23.962 | 1.00 | 36.11 | 7 |
| | ATOM | 3976 | CA | LEU | C | 86 | 33.609 | 62.385 | 25.315 | 1.00 | 36.00 | 6 |
| | ATOM | 3977 | CB | LEU | C | 86 | 32.208 | 61.904 | 25.678 | 1.00 | 35.07 | 6 |
| | ATOM | 3978 | CG | LEU | C | 86 | 31.089 | 62.464 | 24.806 | 1.00 | 36.71 | 6 |
| 25 | ATOM | 3979 | CD1 | LEU | C | 86 | 29.752 | 61.912 | 25.240 | 1.00 | 31.87 | 6 |
| | ATOM | 3980 | CD2 | LEU | C | 86 | 31.112 | 63.974 | 24.910 | 1.00 | 35.41 | 6 |
| | ATOM | 3981 | C | LEU | C | 86 | 34.585 | 61.870 | 26.337 | 1.00 | 36.89 | 6 |
| | ATOM | 3982 | O | LEU | C | 86 | 35.147 | 60.795 | 26.189 | 1.00 | 38.19 | 8 |
| | ATOM | 3983 | N | ALA | C | 87 | 34.773 | 62.648 | 27.391 | 1.00 | 38.71 | 7 |
| 30 | ATOM | 3984 | CA | ALA | C | 87 | 35.672 | 62.268 | 28.461 | 1.00 | 38.06 | 6 |
| | ATOM | 3985 | CB | ALA | C | 87 | 37.045 | 62.838 | 28.200 | 1.00 | 35.59 | 6 |
| | ATOM | 3986 | C | ALA | C | 87 | 35.119 | 62.799 | 29.772 | 1.00 | 38.10 | 6 |
| | ATOM | 3987 | O | ALA | C | 87 | 34.586 | 63.891 | 29.815 | 1.00 | 37.91 | 8 |
| | ATOM | 3988 | N | ALA | C | 88 | 35.217 | 62.013 | 30.833 | 1.00 | 39.52 | 7 |
| 35 | ATOM | 3989 | CA | ALA | C | 88 | 34.756 | 62.448 | 32.147 | 1.00 | 40.05 | 6 |
| | ATOM | 3990 | CB | ALA | C | 88 | 34.356 | 61.250 | 33.005 | 1.00 | 40.30 | 6 |
| | ATOM | 3991 | C | ALA | C | 88 | 35.939 | 63.169 | 32.771 | 1.00 | 41.63 | 6 |
| | ATOM | 3992 | O | ALA | C | 88 | 36.912 | 62.545 | 33.195 | 1.00 | 41.71 | 8 |
| | ATOM | 3993 | N | TYR | C | 89 | 35.852 | 64.492 | 32.799 | 1.00 | 42.71 | 7 |
| 40 | ATOM | 3994 | CA | TYR | C | 89 | 36.904 | 65.350 | 33.330 | 1.00 | 41.60 | 6 |
| | ATOM | 3995 | CB | TYR | C | 89 | 36.368 | 66.775 | 33.459 | 1.00 | 43.41 | 6 |
| | ATOM | 3996 | CG | TYR | C | 89 | 35.976 | 67.422 | 32.149 | 1.00 | 48.68 | 6 |
| | ATOM | 3997 | CD1 | TYR | C | 89 | 35.321 | 68.653 | 32.129 | 1.00 | 51.90 | 6 |
| | ATOM | 3998 | CE1 | TYR | C | 89 | 34.991 | 69.284 | 30.920 | 1.00 | 53.01 | 6 |
| 45 | ATOM | 3999 | CD2 | TYR | C | 89 | 36.290 | 66.830 | 30.929 | 1.00 | 48.32 | 6 |
| | ATOM | 4000 | CE2 | TYR | C | 89 | 35.966 | 67.449 | 29.726 | 1.00 | 52.45 | 6 |
| | ATOM | 4001 | CZ | TYR | C | 89 | 35.318 | 68.678 | 29.730 | 1.00 | 53.45 | 6 |
| | ATOM | 4002 | OH | TYR | C | 89 | 35.017 | 69.305 | 28.545 | 1.00 | 56.75 | 8 |
| | ATOM | 4003 | C | TYR | C | 89 | 37.527 | 64.914 | 34.657 | 1.00 | 40.68 | 6 |
| 50 | ATOM | 4004 | O | TYR | C | 89 | 38.727 | 65.075 | 34.863 | 1.00 | 39.21 | 8 |
| | ATOM | 4005 | N | ASN | C | 90 | 36.725 | 64.364 | 35.562 | 1.00 | 39.53 | 7 |
| | ATOM | 4006 | CA | ASN | C | 90 | 37.265 | 63.952 | 36.848 | 1.00 | 39.15 | 6 |
| | ATOM | 4007 | CB | ASN | C | 90 | 36.476 | 64.603 | 37.989 | 1.00 | 38.99 | 6 |
| | ATOM | 4008 | CG | ASN | C | 90 | 34.995 | 64.290 | 37.944 | 1.00 | 38.22 | 6 |
| 55 | ATOM | 4009 | OD1 | ASN | C | 90 | 34.355 | 64.378 | 36.902 | 1.00 | 37.33 | 8 |
| | ATOM | 4010 | ND2 | ASN | C | 90 | 34.443 | 63.939 | 39.090 | 1.00 | 39.59 | 7 |
| | ATOM | 4011 | C | ASN | C | 90 | 37.343 | 62.448 | 37.033 | 1.00 | 41.22 | 6 |
| | ATOM | 4012 | O | ASN | C | 90 | 37.354 | 61.946 | 38.153 | 1.00 | 42.78 | 8 |
| | ATOM | 4013 | N | ALA | C | 91 | 37.400 | 61.733 | 35.915 | 1.00 | 42.37 | 7 |
| 60 | ATOM | 4014 | CA | ALA | C | 91 | 37.528 | 60.292 | 35.928 | 1.00 | 40.71 | 6 |
| | ATOM | 4015 | CB | ALA | C | 91 | 37.346 | 59.733 | 34.521 | 1.00 | 41.88 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 4016 | C | ALA | C | 91 | 38.939 | 60.033 | 36.435 | 1.00 | 39.96 | 6 |
| | ATOM | 4017 | O | ALA | C | 91 | 39.898 | 60.664 | 36.007 | 1.00 | 35.60 | 8 |
| | ATOM | 4018 | N | ILE | C | 92 | 39.040 | 59.093 | 37.356 | 1.00 | 41.49 | 7 |
| 5 | ATOM | 4019 | CA | ILE | C | 92 | 40.292 | 58.731 | 37.993 | 1.00 | 43.20 | 6 |
| | ATOM | 4020 | CB | ILE | C | 92 | 40.020 | 58.594 | 39.511 | 1.00 | 47.77 | 6 |
| | ATOM | 4021 | CG2 | ILE | C | 92 | 39.923 | 57.130 | 39.921 | 1.00 | 48.36 | 6 |
| | ATOM | 4022 | CG1 | ILE | C | 92 | 41.093 | 59.293 | 40.316 | 1.00 | 50.98 | 6 |
| | ATOM | 4023 | CD1 | ILE | C | 92 | 40.903 | 59.036 | 41.812 | 1.00 | 55.36 | 6 |
| 10 | ATOM | 4024 | C | ILE | C | 92 | 40.861 | 57.416 | 37.403 | 1.00 | 41.81 | 6 |
| | ATOM | 4025 | O | ILE | C | 92 | 41.973 | 56.992 | 37.720 | 1.00 | 40.19 | 8 |
| | ATOM | 4026 | N | SER | C | 93 | 40.080 | 56.781 | 36.541 | 1.00 | 39.24 | 7 |
| | ATOM | 4027 | CA | SER | C | 93 | 40.470 | 55.534 | 35.913 | 1.00 | 39.09 | 6 |
| | ATOM | 4028 | CB | SER | C | 93 | 39.892 | 54.356 | 36.685 | 1.00 | 39.19 | 6 |
| | ATOM | 4029 | OG | SER | C | 93 | 38.479 | 54.310 | 36.541 | 1.00 | 39.34 | 8 |
| 15 | ATOM | 4030 | C | SER | C | 93 | 39.839 | 55.579 | 34.546 | 1.00 | 37.69 | 6 |
| | ATOM | 4031 | O | SER | C | 93 | 38.987 | 56.404 | 34.311 | 1.00 | 39.27 | 8 |
| | ATOM | 4032 | N | LYS | C | 94 | 40.251 | 54.717 | 33.632 | 1.00 | 37.58 | 7 |
| | ATOM | 4033 | CA | LYS | C | 94 | 39.612 | 54.737 | 32.330 | 1.00 | 40.65 | 6 |
| 20 | ATOM | 4034 | CB | LYS | C | 94 | 40.560 | 54.256 | 31.228 | 1.00 | 41.66 | 6 |
| | ATOM | 4035 | CG | LYS | C | 94 | 41.383 | 53.024 | 31.520 | 1.00 | 46.32 | 6 |
| | ATOM | 4036 | CD | LYS | C | 94 | 42.502 | 52.902 | 30.485 | 1.00 | 48.62 | 6 |
| | ATOM | 4037 | CE | LYS | C | 94 | 41.962 | 53.091 | 29.069 | 1.00 | 47.90 | 6 |
| | ATOM | 4038 | NZ | LYS | C | 94 | 42.999 | 52.929 | 28.024 | 1.00 | 48.05 | 7 |
| | ATOM | 4039 | C | LYS | C | 94 | 38.321 | 53.926 | 32.359 | 1.00 | 40.78 | 6 |
| 25 | ATOM | 4040 | O | LYS | C | 94 | 38.102 | 53.094 | 33.234 | 1.00 | 42.52 | 8 |
| | ATOM | 4041 | N | PRO | C | 95 | 37.434 | 54.178 | 31.404 | 1.00 | 41.55 | 7 |
| | ATOM | 4042 | CD | PRO | C | 95 | 37.555 | 55.150 | 30.312 | 1.00 | 42.12 | 6 |
| | ATOM | 4043 | CA | PRO | C | 95 | 36.153 | 53.479 | 31.335 | 1.00 | 41.34 | 6 |
| | ATOM | 4044 | CB | PRO | C | 95 | 35.439 | 54.166 | 30.177 | 1.00 | 41.08 | 6 |
| 30 | ATOM | 4045 | CG | PRO | C | 95 | 36.125 | 55.476 | 30.058 | 1.00 | 42.87 | 6 |
| | ATOM | 4046 | C | PRO | C | 95 | 36.256 | 52.000 | 31.102 | 1.00 | 40.86 | 6 |
| | ATOM | 4047 | O | PRO | C | 95 | 36.941 | 51.563 | 30.189 | 1.00 | 41.65 | 8 |
| | ATOM | 4048 | N | GLU | C | 96 | 35.581 | 51.228 | 31.940 | 1.00 | 40.55 | 7 |
| | ATOM | 4049 | CA | GLU | C | 96 | 35.560 | 49.791 | 31.766 | 1.00 | 41.10 | 6 |
| 35 | ATOM | 4050 | CB | GLU | C | 96 | 35.684 | 49.050 | 33.104 | 1.00 | 43.71 | 6 |
| | ATOM | 4051 | CG | GLU | C | 96 | 35.762 | 47.521 | 32.954 | 1.00 | 49.85 | 6 |
| | ATOM | 4052 | CD | GLU | C | 96 | 35.912 | 46.768 | 34.286 | 1.00 | 54.35 | 6 |
| | ATOM | 4053 | OE1 | GLU | C | 96 | 36.282 | 47.404 | 35.302 | 1.00 | 58.62 | 8 |
| | ATOM | 4054 | OE2 | GLU | C | 96 | 35.682 | 45.534 | 34.316 | 1.00 | 52.48 | 8 |
| 40 | ATOM | 4055 | C | GLU | C | 96 | 34.190 | 49.553 | 31.168 | 1.00 | 39.91 | 6 |
| | ATOM | 4056 | O | GLU | C | 96 | 33.200 | 49.478 | 31.894 | 1.00 | 40.62 | 8 |
| | ATOM | 4057 | N | VAL | C | 97 | 34.133 | 49.483 | 29.841 | 1.00 | 35.73 | 7 |
| | ATOM | 4058 | CA | VAL | C | 97 | 32.876 | 49.249 | 29.153 | 1.00 | 34.27 | 6 |
| | ATOM | 4059 | CB | VAL | C | 97 | 33.006 | 49.541 | 27.660 | 1.00 | 31.66 | 6 |
| 45 | ATOM | 4060 | CG1 | VAL | C | 97 | 31.686 | 49.333 | 26.968 | 1.00 | 34.09 | 6 |
| | ATOM | 4061 | CG2 | VAL | C | 97 | 33.437 | 50.963 | 27.470 | 1.00 | 30.22 | 6 |
| | ATOM | 4062 | C | VAL | C | 97 | 32.481 | 47.801 | 29.382 | 1.00 | 34.55 | 6 |
| | ATOM | 4063 | O | VAL | C | 97 | 33.167 | 46.891 | 28.949 | 1.00 | 35.63 | 8 |
| | ATOM | 4064 | N | LEU | C | 98 | 31.362 | 47.607 | 30.072 | 1.00 | 35.35 | 7 |
| 50 | ATOM | 4065 | CA | LEU | C | 98 | 30.868 | 46.286 | 30.433 | 1.00 | 34.12 | 6 |
| | ATOM | 4066 | CB | LEU | C | 98 | 30.098 | 46.377 | 31.752 | 1.00 | 33.63 | 6 |
| | ATOM | 4067 | CG | LEU | C | 98 | 30.741 | 47.049 | 32.961 | 1.00 | 35.44 | 6 |
| | ATOM | 4068 | CD1 | LEU | C | 98 | 29.694 | 47.352 | 33.989 | 1.00 | 37.77 | 6 |
| | ATOM | 4069 | CD2 | LEU | C | 98 | 31.806 | 46.166 | 33.538 | 1.00 | 34.23 | 6 |
| 55 | ATOM | 4070 | C | LEU | C | 98 | 29.965 | 45.641 | 29.404 | 1.00 | 36.94 | 6 |
| | ATOM | 4071 | O | LEU | C | 98 | 29.640 | 44.464 | 29.524 | 1.00 | 39.49 | 8 |
| | ATOM | 4072 | N | THR | C | 99 | 29.567 | 46.398 | 28.389 | 1.00 | 36.94 | 7 |
| | ATOM | 4073 | CA | THR | C | 99 | 28.642 | 45.881 | 27.393 | 1.00 | 36.72 | 6 |
| | ATOM | 4074 | CB | THR | C | 99 | 27.317 | 46.674 | 27.450 | 1.00 | 36.81 | 6 |
| 60 | ATOM | 4075 | OG1 | THR | C | 99 | 27.574 | 48.076 | 27.259 | 1.00 | 40.25 | 8 |
| | ATOM | 4076 | CG2 | THR | C | 99 | 26.648 | 46.474 | 28.792 | 1.00 | 34.14 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 4077 | C | THR | C | 99 | 29.154 | 45.895 | 25.965 | 1.00 | 37.65 | 6 |
| | ATOM | 4078 | O | THR | C | 99 | 30.147 | 46.549 | 25.664 | 1.00 | 37.93 | 8 |
| | ATOM | 4079 | N | PRO | C | 100 | 28.497 | 45.134 | 25.073 | 1.00 | 37.89 | 7 |
| 5 | ATOM | 4080 | CD | PRO | C | 100 | 27.443 | 44.145 | 25.364 | 1.00 | 40.71 | 6 |
| | ATOM | 4081 | CA | PRO | C | 100 | 28.874 | 45.065 | 23.667 | 1.00 | 37.03 | 6 |
| | ATOM | 4082 | CB | PRO | C | 100 | 27.716 | 44.298 | 23.046 | 1.00 | 37.46 | 6 |
| | ATOM | 4083 | CG | PRO | C | 100 | 27.402 | 43.316 | 24.094 | 1.00 | 38.27 | 6 |
| | ATOM | 4084 | C | PRO | C | 100 | 28.963 | 46.476 | 23.139 | 1.00 | 38.41 | 6 |
| | ATOM | 4085 | O | PRO | C | 100 | 28.082 | 47.297 | 23.390 | 1.00 | 39.24 | 8 |
| 10 | ATOM | 4086 | N | GLN | C | 101 | 30.026 | 46.772 | 22.412 | 1.00 | 38.06 | 7 |
| | ATOM | 4087 | CA | GLN | C | 101 | 30.169 | 48.113 | 21.893 | 1.00 | 39.24 | 6 |
| | ATOM | 4088 | CB | GLN | C | 101 | 31.639 | 48.479 | 21.827 | 1.00 | 38.35 | 6 |
| | ATOM | 4089 | CG | GLN | C | 101 | 32.140 | 48.846 | 23.195 | 1.00 | 43.58 | 6 |
| | ATOM | 4090 | CD | GLN | C | 101 | 33.633 | 48.822 | 23.291 | 1.00 | 47.06 | 6 |
| 15 | ATOM | 4091 | OE1 | GLN | C | 101 | 34.315 | 49.497 | 22.533 | 1.00 | 51.61 | 8 |
| | ATOM | 4092 | NE2 | GLN | C | 101 | 34.160 | 48.041 | 24.227 | 1.00 | 48.13 | 7 |
| | ATOM | 4093 | C | GLN | C | 101 | 29.471 | 48.333 | 20.571 | 1.00 | 38.37 | 6 |
| | ATOM | 4094 | O | GLN | C | 101 | 30.095 | 48.620 | 19.554 | 1.00 | 36.55 | 8 |
| | ATOM | 4095 | N | LEU | C | 102 | 28.148 | 48.198 | 20.627 | 1.00 | 40.04 | 7 |
| 20 | ATOM | 4096 | CA | LEU | C | 102 | 27.263 | 48.373 | 19.478 | 1.00 | 40.82 | 6 |
| | ATOM | 4097 | CB | LEU | C | 102 | 26.376 | 47.143 | 19.289 | 1.00 | 38.65 | 6 |
| | ATOM | 4098 | CG | LEU | C | 102 | 27.061 | 45.791 | 19.163 | 1.00 | 40.16 | 6 |
| | ATOM | 4099 | CD1 | LEU | C | 102 | 26.015 | 44.708 | 18.994 | 1.00 | 37.69 | 6 |
| | ATOM | 4100 | CD2 | LEU | C | 102 | 27.991 | 45.815 | 17.981 | 1.00 | 39.89 | 6 |
| 25 | ATOM | 4101 | C | LEU | C | 102 | 26.362 | 49.583 | 19.685 | 1.00 | 40.48 | 6 |
| | ATOM | 4102 | O | LEU | C | 102 | 25.940 | 49.880 | 20.800 | 1.00 | 39.50 | 8 |
| | ATOM | 4103 | N | ALA | C | 103 | 26.072 | 50.280 | 18.603 | 1.00 | 40.58 | 7 |
| | ATOM | 4104 | CA | ALA | C | 103 | 25.203 | 51.434 | 18.674 | 1.00 | 42.17 | 6 |
| | ATOM | 4105 | CB | ALA | C | 103 | 25.879 | 52.646 | 18.054 | 1.00 | 43.90 | 6 |
| 30 | ATOM | 4106 | C | ALA | C | 103 | 23.950 | 51.087 | 17.904 | 1.00 | 43.55 | 6 |
| | ATOM | 4107 | O | ALA | C | 103 | 23.905 | 50.092 | 17.189 | 1.00 | 44.89 | 8 |
| | ATOM | 4108 | N | ARG | C | 104 | 22.930 | 51.916 | 18.048 | 1.00 | 45.38 | 7 |
| | ATOM | 4109 | CA | ARG | C | 104 | 21.674 | 51.689 | 17.359 | 1.00 | 46.54 | 6 |
| | ATOM | 4110 | CB | ARG | C | 104 | 20.549 | 51.665 | 18.381 | 1.00 | 46.10 | 6 |
| 35 | ATOM | 4111 | CG | ARG | C | 104 | 19.292 | 51.040 | 17.879 | 1.00 | 47.91 | 6 |
| | ATOM | 4112 | CD | ARG | C | 104 | 19.457 | 49.560 | 17.559 | 1.00 | 45.29 | 6 |
| | ATOM | 4113 | NE | ARG | C | 104 | 18.188 | 49.059 | 17.035 | 1.00 | 46.68 | 7 |
| | ATOM | 4114 | CZ | ARG | C | 104 | 17.927 | 47.792 | 16.761 | 1.00 | 46.66 | 6 |
| | ATOM | 4115 | NH1 | ARG | C | 104 | 18.850 | 46.866 | 16.954 | 1.00 | 47.05 | 7 |
| 40 | ATOM | 4116 | NH2 | ARG | C | 104 | 16.733 | 47.452 | 16.308 | 1.00 | 48.97 | 7 |
| | ATOM | 4117 | C | ARG | C | 104 | 21.491 | 52.830 | 16.367 | 1.00 | 46.82 | 6 |
| | ATOM | 4118 | O | ARG | C | 104 | 21.550 | 53.999 | 16.738 | 1.00 | 49.29 | 8 |
| | ATOM | 4119 | N | VAL | C | 105 | 21.296 | 52.501 | 15.098 | 1.00 | 47.65 | 7 |
| | ATOM | 4120 | CA | VAL | C | 105 | 21.138 | 53.543 | 14.092 | 1.00 | 47.99 | 6 |
| 45 | ATOM | 4121 | CB | VAL | C | 105 | 22.200 | 53.426 | 12.980 | 1.00 | 46.29 | 6 |
| | ATOM | 4122 | CG1 | VAL | C | 105 | 22.080 | 54.588 | 12.021 | 1.00 | 44.96 | 6 |
| | ATOM | 4123 | CG2 | VAL | C | 105 | 23.583 | 53.386 | 13.580 | 1.00 | 42.95 | 6 |
| | ATOM | 4124 | C | VAL | C | 105 | 19.769 | 53.519 | 13.444 | 1.00 | 50.20 | 6 |
| | ATOM | 4125 | O | VAL | C | 105 | 19.340 | 52.497 | 12.904 | 1.00 | 50.01 | 8 |
| 50 | ATOM | 4126 | N | VAL | C | 106 | 19.097 | 54.666 | 13.506 | 1.00 | 51.90 | 7 |
| | ATOM | 4127 | CA | VAL | C | 106 | 17.767 | 54.836 | 12.933 | 1.00 | 53.33 | 6 |
| | ATOM | 4128 | CB | VAL | C | 106 | 16.947 | 55.840 | 13.758 | 1.00 | 51.93 | 6 |
| | ATOM | 4129 | CG1 | VAL | C | 106 | 15.503 | 55.825 | 13.306 | 1.00 | 49.94 | 6 |
| | ATOM | 4130 | CG2 | VAL | C | 106 | 17.060 | 55.504 | 15.222 | 1.00 | 50.56 | 6 |
| 55 | ATOM | 4131 | C | VAL | C | 106 | 17.899 | 55.347 | 11.497 | 1.00 | 53.76 | 6 |
| | ATOM | 4132 | O | VAL | C | 106 | 18.782 | 56.151 | 11.203 | 1.00 | 52.33 | 8 |
| | ATOM | 4133 | N | SER | C | 107 | 17.016 | 54.889 | 10.615 | 1.00 | 54.08 | 7 |
| | ATOM | 4134 | CA | SER | C | 107 | 17.066 | 55.275 | 9.208 | 1.00 | 56.13 | 6 |
| | ATOM | 4135 | CB | SER | C | 107 | 15.835 | 54.734 | 8.487 | 1.00 | 56.67 | 6 |
| 60 | ATOM | 4136 | OG | SER | C | 107 | 14.672 | 54.943 | 9.268 | 1.00 | 59.41 | 8 |
| | ATOM | 4137 | C | SER | C | 107 | 17.228 | 56.762 | 8.895 | 1.00 | 56.30 | 6 |

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|----|------|------|---------------|--------|--------|--------|------|-------|----|--|
| 5 | ATOM | 4138 | O SER C 107 | 17.678 | 57.129 | 7.797 | 1.00 | 55.13 | 8 | |
| | ATOM | 4139 | N ASP C 108 | 16.879 | 57.619 | 9.849 | 1.00 | 56.72 | 7 | |
| | ATOM | 4140 | CA ASP C 108 | 16.999 | 59.064 | 9.632 | 1.00 | 58.46 | 6 | |
| | ATOM | 4141 | CB ASP C 108 | 15.875 | 59.807 | 10.353 | 1.00 | 59.64 | 6 | |
| | ATOM | 4142 | CG ASP C 108 | 15.998 | 59.735 | 11.856 | 1.00 | 60.59 | 6 | |
| 10 | ATOM | 4143 | OD1 ASP C 108 | 16.432 | 58.693 | 12.378 | 1.00 | 61.80 | 8 | |
| | ATOM | 4144 | OD2 ASP C 108 | 15.643 | 60.724 | 12.520 | 1.00 | 63.04 | 8 | |
| | ATOM | 4145 | C ASP C 108 | 18.345 | 59.648 | 10.054 | 1.00 | 58.38 | 6 | |
| | ATOM | 4146 | O ASP C 108 | 18.513 | 60.859 | 10.068 | 1.00 | 58.33 | 8 | |
| | ATOM | 4147 | N GLY C 109 | 19.299 | 58.785 | 10.396 | 1.00 | 59.41 | 7 | |
| 15 | ATOM | 4148 | CA GLY C 109 | 20.618 | 59.246 | 10.786 | 1.00 | 58.66 | 6 | |
| | ATOM | 4149 | C GLY C 109 | 20.802 | 59.467 | 12.271 | 1.00 | 59.58 | 6 | |
| | ATOM | 4150 | O GLY C 109 | 21.868 | 59.926 | 12.695 | 1.00 | 59.07 | 8 | |
| | ATOM | 4151 | N GLU C 110 | 19.775 | 59.165 | 13.064 | 1.00 | 59.04 | 7 | |
| | ATOM | 4152 | CA GLU C 110 | 19.871 | 59.325 | 14.508 | 1.00 | 59.38 | 6 | |
| 20 | ATOM | 4153 | CB GLU C 110 | 18.481 | 59.327 | 15.141 | 1.00 | 62.39 | 6 | |
| | ATOM | 4154 | CG GLU C 110 | 18.386 | 60.020 | 16.513 | 1.00 | 66.23 | 6 | |
| | ATOM | 4155 | CD GLU C 110 | 18.717 | 61.520 | 16.441 | 1.00 | 70.42 | 6 | |
| | ATOM | 4156 | OE1 GLU C 110 | 18.640 | 62.107 | 15.333 | 1.00 | 69.27 | 8 | |
| | ATOM | 4157 | OE2 GLU C 110 | 19.047 | 62.117 | 17.493 | 1.00 | 72.25 | 8 | |
| 25 | ATOM | 4158 | C GLU C 110 | 20.677 | 58.141 | 15.038 | 1.00 | 59.61 | 6 | |
| | ATOM | 4159 | O GLU C 110 | 20.467 | 56.995 | 14.623 | 1.00 | 60.95 | 8 | |
| | ATOM | 4160 | N VAL C 111 | 21.600 | 58.419 | 15.953 | 1.00 | 57.63 | 7 | |
| | ATOM | 4161 | CA VAL C 111 | 22.444 | 57.379 | 16.535 | 1.00 | 55.43 | 6 | |
| | ATOM | 4162 | CB VAL C 111 | 23.926 | 57.620 | 16.200 | 1.00 | 55.71 | 6 | |
| 30 | ATOM | 4163 | CG1 VAL C 111 | 24.783 | 56.511 | 16.788 | 1.00 | 53.14 | 6 | |
| | ATOM | 4164 | CG2 VAL C 111 | 24.105 | 57.706 | 14.686 | 1.00 | 56.04 | 6 | |
| | ATOM | 4165 | C VAL C 111 | 22.308 | 57.337 | 18.048 | 1.00 | 54.63 | 6 | |
| | ATOM | 4166 | O VAL C 111 | 22.328 | 58.373 | 18.706 | 1.00 | 53.67 | 8 | |
| | ATOM | 4167 | N LEU C 112 | 22.171 | 56.137 | 18.596 | 1.00 | 53.09 | 7 | |
| 35 | ATOM | 4168 | CA LEU C 112 | 22.050 | 55.992 | 20.034 | 1.00 | 53.62 | 6 | |
| | ATOM | 4169 | CB LEU C 112 | 20.638 | 55.548 | 20.420 | 1.00 | 56.64 | 6 | |
| | ATOM | 4170 | CG LEU C 112 | 19.380 | 56.011 | 19.657 | 1.00 | 60.85 | 6 | |
| | ATOM | 4171 | CD1 LEU C 112 | 19.439 | 57.490 | 19.341 | 1.00 | 62.41 | 6 | |
| | ATOM | 4172 | CD2 LEU C 112 | 19.244 | 55.207 | 18.374 | 1.00 | 62.32 | 6 | |
| 40 | ATOM | 4173 | C LEU C 112 | 23.053 | 54.963 | 20.542 | 1.00 | 53.28 | 6 | |
| | ATOM | 4174 | O LEU C 112 | 23.024 | 53.807 | 20.134 | 1.00 | 54.91 | 8 | |
| | ATOM | 4175 | N TYR C 113 | 23.943 | 55.389 | 21.429 | 1.00 | 50.87 | 7 | |
| | ATOM | 4176 | CA TYR C 113 | 24.947 | 54.502 | 22.003 | 1.00 | 47.87 | 6 | |
| | ATOM | 4177 | CB TYR C 113 | 26.362 | 54.924 | 21.560 | 1.00 | 44.85 | 6 | |
| 45 | ATOM | 4178 | CG TYR C 113 | 27.500 | 54.099 | 22.134 | 1.00 | 40.84 | 6 | |
| | ATOM | 4179 | CD1 TYR C 113 | 27.428 | 52.716 | 22.181 | 1.00 | 39.92 | 6 | |
| | ATOM | 4180 | CE1 TYR C 113 | 28.481 | 51.956 | 22.679 | 1.00 | 39.26 | 6 | |
| | ATOM | 4181 | CD2 TYR C 113 | 28.663 | 54.710 | 22.602 | 1.00 | 41.11 | 6 | |
| | ATOM | 4182 | CE2 TYR C 113 | 29.720 | 53.962 | 23.100 | 1.00 | 40.68 | 6 | |
| 50 | ATOM | 4183 | CZ TYR C 113 | 29.625 | 52.583 | 23.138 | 1.00 | 41.46 | 6 | |
| | ATOM | 4184 | OH TYR C 113 | 30.667 | 51.831 | 23.649 | 1.00 | 40.70 | 8 | |
| | ATOM | 4185 | C TYR C 113 | 24.805 | 54.611 | 23.508 | 1.00 | 48.03 | 6 | |
| | ATOM | 4186 | O TYR C 113 | 25.002 | 55.673 | 24.089 | 1.00 | 47.83 | 8 | |
| | ATOM | 4187 | N MET C 114 | 24.457 | 53.508 | 24.146 | 1.00 | 48.88 | 7 | |
| 55 | ATOM | 4188 | CA MET C 114 | 24.283 | 53.519 | 25.583 | 1.00 | 49.26 | 6 | |
| | ATOM | 4189 | CB MET C 114 | 22.809 | 53.375 | 25.910 | 1.00 | 53.64 | 6 | |
| | ATOM | 4190 | CG MET C 114 | 22.494 | 53.558 | 27.370 | 1.00 | 58.33 | 6 | |
| | ATOM | 4191 | SD MET C 114 | 20.864 | 52.927 | 27.696 | 1.00 | 67.34 | 16 | |
| | ATOM | 4192 | CE MET C 114 | 19.859 | 54.330 | 27.098 | 1.00 | 65.99 | 6 | |
| 60 | ATOM | 4193 | C MET C 114 | 25.055 | 52.393 | 26.244 | 1.00 | 47.94 | 6 | |
| | ATOM | 4194 | O MET C 114 | 24.485 | 51.360 | 26.579 | 1.00 | 48.32 | 8 | |
| | ATOM | 4195 | N PRO C 115 | 26.364 | 52.576 | 26.440 | 1.00 | 47.40 | 7 | |
| | ATOM | 4196 | CD PRO C 115 | 27.181 | 53.711 | 25.976 | 1.00 | 49.35 | 6 | |
| | ATOM | 4197 | CA PRO C 115 | 27.207 | 51.556 | 27.066 | 1.00 | 48.05 | 6 | |
| | ATOM | 4198 | CB PRO C 115 | 28.591 | 51.903 | 26.545 | 1.00 | 48.90 | 6 | |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 4199 | CG | PRO | C | 115 | 28.548 | 53.398 | 26.559 | 1.00 | 48.59 | 6 |
| | ATOM | 4200 | C | PRO | C | 115 | 27.153 | 51.636 | 28.585 | 1.00 | 48.68 | 6 |
| | ATOM | 4201 | O | PRO | C | 115 | 26.976 | 52.720 | 29.142 | 1.00 | 48.78 | 8 |
| | ATOM | 4202 | N | SER | C | 116 | 27.291 | 50.493 | 29.249 | 1.00 | 47.05 | 7 |
| 5 | ATOM | 4203 | CA | SER | C | 116 | 27.292 | 50.481 | 30.699 | 1.00 | 45.85 | 6 |
| | ATOM | 4204 | CB | SER | C | 116 | 26.746 | 49.178 | 31.248 | 1.00 | 45.70 | 6 |
| | ATOM | 4205 | OG | SER | C | 116 | 26.731 | 49.228 | 32.667 | 1.00 | 46.59 | 8 |
| | ATOM | 4206 | C | SER | C | 116 | 28.743 | 50.607 | 31.097 | 1.00 | 47.30 | 6 |
| | ATOM | 4207 | O | SER | C | 116 | 29.568 | 49.794 | 30.695 | 1.00 | 48.38 | 8 |
| 10 | ATOM | 4208 | N | ILE | C | 117 | 29.058 | 51.622 | 31.892 | 1.00 | 45.86 | 7 |
| | ATOM | 4209 | CA | ILE | C | 117 | 30.437 | 51.849 | 32.293 | 1.00 | 41.61 | 6 |
| | ATOM | 4210 | CB | ILE | C | 117 | 30.926 | 53.210 | 31.749 | 1.00 | 39.60 | 6 |
| | ATOM | 4211 | CG2 | ILE | C | 117 | 32.325 | 53.499 | 32.230 | 1.00 | 38.47 | 6 |
| | ATOM | 4212 | CG1 | ILE | C | 117 | 30.876 | 53.208 | 30.225 | 1.00 | 38.60 | 6 |
| 15 | ATOM | 4213 | CD1 | ILE | C | 117 | 31.025 | 54.563 | 29.619 | 1.00 | 34.54 | 6 |
| | ATOM | 4214 | C | ILE | C | 117 | 30.708 | 51.830 | 33.796 | 1.00 | 42.04 | 6 |
| | ATOM | 4215 | O | ILE | C | 117 | 29.948 | 52.390 | 34.587 | 1.00 | 42.87 | 8 |
| | ATOM | 4216 | N | ARG | C | 118 | 31.787 | 51.158 | 34.182 | 1.00 | 40.79 | 7 |
| | ATOM | 4217 | CA | ARG | C | 118 | 32.210 | 51.162 | 35.568 | 1.00 | 40.35 | 6 |
| 20 | ATOM | 4218 | CB | ARG | C | 118 | 32.607 | 49.782 | 36.060 | 1.00 | 37.23 | 6 |
| | ATOM | 4219 | CG | ARG | C | 118 | 33.172 | 49.866 | 37.455 | 1.00 | 36.55 | 6 |
| | ATOM | 4220 | CD | ARG | C | 118 | 33.277 | 48.538 | 38.156 | 1.00 | 39.03 | 6 |
| | ATOM | 4221 | NE | ARG | C | 118 | 33.874 | 48.693 | 39.483 | 1.00 | 39.42 | 7 |
| | ATOM | 4222 | CZ | ARG | C | 118 | 33.882 | 47.756 | 40.424 | 1.00 | 39.50 | 6 |
| 25 | ATOM | 4223 | NH1 | ARG | C | 118 | 33.326 | 46.574 | 40.208 | 1.00 | 40.01 | 7 |
| | ATOM | 4224 | NH2 | ARG | C | 118 | 34.434 | 48.012 | 41.594 | 1.00 | 40.75 | 7 |
| | ATOM | 4225 | C | ARG | C | 118 | 33.440 | 52.065 | 35.545 | 1.00 | 41.99 | 6 |
| | ATOM | 4226 | O | ARG | C | 118 | 34.322 | 51.881 | 34.722 | 1.00 | 43.88 | 8 |
| | ATOM | 4227 | N | GLN | C | 119 | 33.514 | 53.040 | 36.436 | 1.00 | 42.79 | 7 |
| 30 | ATOM | 4228 | CA | GLN | C | 119 | 34.649 | 53.947 | 36.408 | 1.00 | 43.05 | 6 |
| | ATOM | 4229 | CB | GLN | C | 119 | 34.439 | 54.914 | 35.252 | 1.00 | 41.88 | 6 |
| | ATOM | 4230 | CG | GLN | C | 119 | 35.502 | 55.939 | 35.034 | 1.00 | 41.06 | 6 |
| | ATOM | 4231 | CD | GLN | C | 119 | 35.281 | 56.668 | 33.732 | 1.00 | 41.03 | 6 |
| | ATOM | 4232 | OE1 | GLN | C | 119 | 34.148 | 56.899 | 33.331 | 1.00 | 40.46 | 8 |
| 35 | ATOM | 4233 | NE2 | GLN | C | 119 | 36.363 | 57.039 | 33.066 | 1.00 | 43.78 | 7 |
| | ATOM | 4234 | C | GLN | C | 119 | 34.786 | 54.685 | 37.728 | 1.00 | 43.66 | 6 |
| | ATOM | 4235 | O | GLN | C | 119 | 33.803 | 54.937 | 38.397 | 1.00 | 45.00 | 8 |
| | ATOM | 4236 | N | ARG | C | 120 | 36.008 | 55.018 | 38.113 | 1.00 | 44.71 | 7 |
| | ATOM | 4237 | CA | ARG | C | 120 | 36.210 | 55.722 | 39.369 | 1.00 | 48.39 | 6 |
| 40 | ATOM | 4238 | CB | ARG | C | 120 | 37.414 | 55.169 | 40.107 | 1.00 | 51.11 | 6 |
| | ATOM | 4239 | CG | ARG | C | 120 | 37.325 | 53.696 | 40.397 | 1.00 | 56.82 | 6 |
| | ATOM | 4240 | CD | ARG | C | 120 | 38.116 | 53.386 | 41.641 | 1.00 | 64.45 | 6 |
| | ATOM | 4241 | NE | ARG | C | 120 | 37.375 | 53.650 | 42.886 | 1.00 | 68.42 | 7 |
| | ATOM | 4242 | CZ | ARG | C | 120 | 37.903 | 54.231 | 43.969 | 1.00 | 68.95 | 6 |
| 45 | ATOM | 4243 | NH1 | ARG | C | 120 | 39.169 | 54.631 | 43.967 | 1.00 | 66.80 | 7 |
| | ATOM | 4244 | NH2 | ARG | C | 120 | 37.177 | 54.373 | 45.076 | 1.00 | 69.05 | 7 |
| | ATOM | 4245 | C | ARG | C | 120 | 36.388 | 57.215 | 39.168 | 1.00 | 48.49 | 6 |
| | ATOM | 4246 | O | ARG | C | 120 | 36.937 | 57.660 | 38.161 | 1.00 | 48.13 | 8 |
| | ATOM | 4247 | N | PHE | C | 121 | 35.916 | 57.992 | 40.133 | 1.00 | 47.70 | 7 |
| 50 | ATOM | 4248 | CA | PHE | C | 121 | 36.013 | 59.437 | 40.035 | 1.00 | 47.31 | 6 |
| | ATOM | 4249 | CB | PHE | C | 121 | 34.649 | 60.045 | 39.719 | 1.00 | 43.68 | 6 |
| | ATOM | 4250 | CG | PHE | C | 121 | 34.022 | 59.489 | 38.504 | 1.00 | 43.63 | 6 |
| | ATOM | 4251 | CD1 | PHE | C | 121 | 33.365 | 58.275 | 38.549 | 1.00 | 42.29 | 6 |
| | ATOM | 4252 | CD2 | PHE | C | 121 | 34.104 | 60.165 | 37.301 | 1.00 | 44.87 | 6 |
| 55 | ATOM | 4253 | CE1 | PHE | C | 121 | 32.793 | 57.741 | 37.410 | 1.00 | 44.63 | 6 |
| | ATOM | 4254 | CE2 | PHE | C | 121 | 33.539 | 59.643 | 36.160 | 1.00 | 45.50 | 6 |
| | ATOM | 4255 | CZ | PHE | C | 121 | 32.878 | 58.425 | 36.213 | 1.00 | 45.14 | 6 |
| | ATOM | 4256 | C | PHE | C | 121 | 36.535 | 60.098 | 41.280 | 1.00 | 46.67 | 6 |
| | ATOM | 4257 | O | PHE | C | 121 | 36.528 | 59.525 | 42.359 | 1.00 | 47.10 | 8 |
| 60 | ATOM | 4258 | N | SER | C | 122 | 36.984 | 61.328 | 41.098 | 1.00 | 47.71 | 7 |
| | ATOM | 4259 | CA | SER | C | 122 | 37.469 | 62.150 | 42.187 | 1.00 | 49.70 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|----------|
| 5 | ATOM | 4260 | CB | SER C 122 | 38.799 | 62.808 | 41.809 | 1.00 | 51.31 6 |
| | ATOM | 4261 | OG | SER C 122 | 39.240 | 63.688 | 42.829 | 1.00 | 51.16 8 |
| | ATOM | 4262 | C | SER C 122 | 36.387 | 63.213 | 42.365 | 1.00 | 50.12 6 |
| | ATOM | 4263 | O | SER C 122 | 36.169 | 64.050 | 41.489 | 1.00 | 49.00 8 |
| | ATOM | 4264 | N | CYS C 123 | 35.687 | 63.156 | 43.488 | 1.00 | 50.55 7 |
| | ATOM | 4265 | CA | CYS C 123 | 34.636 | 64.112 | 43.754 | 1.00 | 52.50 6 |
| | ATOM | 4266 | C | CYS C 123 | 34.356 | 64.198 | 45.246 | 1.00 | 54.52 6 |
| | ATOM | 4267 | O | CYS C 123 | 34.998 | 63.514 | 46.043 | 1.00 | 54.24 8 |
| 10 | ATOM | 4268 | CB | CYS C 123 | 33.377 | 63.709 | 42.993 | 1.00 | 53.16 6 |
| | ATOM | 4269 | SG | CYS C 123 | 32.811 | 62.031 | 43.374 | 1.00 | 51.95 16 |
| | ATOM | 4270 | N | ASP C 124 | 33.389 | 65.037 | 45.622 | 1.00 | 56.86 7 |
| | ATOM | 4271 | CA | ASP C 124 | 33.047 | 65.215 | 47.034 | 1.00 | 58.55 6 |
| 15 | ATOM | 4272 | CB | ASP C 124 | 32.265 | 66.514 | 47.252 | 1.00 | 58.22 6 |
| | ATOM | 4273 | CG | ASP C 124 | 32.506 | 67.105 | 48.634 | 1.00 | 58.91 6 |
| | ATOM | 4274 | OD1 | ASP C 124 | 32.703 | 66.338 | 49.589 | 1.00 | 58.22 8 |
| | ATOM | 4275 | OD2 | ASP C 124 | 32.500 | 68.341 | 48.777 | 1.00 | 62.67 8 |
| | ATOM | 4276 | C | ASP C 124 | 32.246 | 64.055 | 47.601 | 1.00 | 58.49 6 |
| | ATOM | 4277 | O | ASP C 124 | 31.098 | 63.837 | 47.229 | 1.00 | 58.26 8 |
| 20 | ATOM | 4278 | N | VAL C 125 | 32.868 | 63.320 | 48.513 | 1.00 | 59.01 7 |
| | ATOM | 4279 | CA | VAL C 125 | 32.232 | 62.175 | 49.152 | 1.00 | 60.88 6 |
| | ATOM | 4280 | CB | VAL C 125 | 33.224 | 60.983 | 49.243 | 1.00 | 59.28 6 |
| | ATOM | 4281 | CG1 | VAL C 125 | 32.601 | 59.838 | 49.983 | 1.00 | 56.75 6 |
| | ATOM | 4282 | CG2 | VAL C 125 | 33.639 | 60.552 | 47.856 | 1.00 | 58.31 6 |
| | ATOM | 4283 | C | VAL C 125 | 31.740 | 62.530 | 50.565 | 1.00 | 63.26 6 |
| 25 | ATOM | 4284 | O | VAL C 125 | 30.892 | 61.833 | 51.143 | 1.00 | 63.90 8 |
| | ATOM | 4285 | N | SER C 126 | 32.267 | 63.616 | 51.122 | 1.00 | 63.98 7 |
| | ATOM | 4286 | CA | SER C 126 | 31.878 | 64.026 | 52.464 | 1.00 | 64.49 6 |
| | ATOM | 4287 | CB | SER C 126 | 32.464 | 65.400 | 52.793 | 1.00 | 63.93 6 |
| 30 | ATOM | 4288 | OG | SER C 126 | 31.972 | 66.381 | 51.898 | 1.00 | 61.34 8 |
| | ATOM | 4289 | C | SER C 126 | 30.364 | 64.061 | 52.614 | 1.00 | 64.90 6 |
| | ATOM | 4290 | O | SER C 126 | 29.654 | 64.603 | 51.766 | 1.00 | 64.08 8 |
| | ATOM | 4291 | N | GLY C 127 | 29.871 | 63.458 | 53.689 | 1.00 | 66.05 7 |
| | ATOM | 4292 | CA | GLY C 127 | 28.442 | 63.458 | 53.929 | 1.00 | 68.25 6 |
| | ATOM | 4293 | C | GLY C 127 | 27.742 | 62.201 | 53.467 | 1.00 | 69.88 6 |
| 35 | ATOM | 4294 | O | GLY C 127 | 26.546 | 62.040 | 53.679 | 1.00 | 70.57 8 |
| | ATOM | 4295 | N | VAL C 128 | 28.480 | 61.297 | 52.839 | 1.00 | 71.23 7 |
| | ATOM | 4296 | CA | VAL C 128 | 27.871 | 60.065 | 52.366 | 1.00 | 72.78 6 |
| | ATOM | 4297 | CB | VAL C 128 | 28.890 | 59.124 | 51.690 | 1.00 | 72.13 6 |
| 40 | ATOM | 4298 | CG1 | VAL C 128 | 29.282 | 59.670 | 50.361 | 1.00 | 75.47 6 |
| | ATOM | 4299 | CG2 | VAL C 128 | 30.104 | 58.940 | 52.585 | 1.00 | 70.24 6 |
| | ATOM | 4300 | C | VAL C 128 | 27.223 | 59.242 | 53.466 | 1.00 | 74.00 6 |
| | ATOM | 4301 | O | VAL C 128 | 26.090 | 58.770 | 53.316 | 1.00 | 73.73 8 |
| 45 | ATOM | 4302 | N | ASP C 129 | 27.946 | 59.063 | 54.567 | 1.00 | 75.39 7 |
| | ATOM | 4303 | CA | ASP C 129 | 27.440 | 58.222 | 55.628 | 1.00 | 77.33 6 |
| | ATOM | 4304 | CB | ASP C 129 | 28.490 | 58.040 | 56.721 | 1.00 | 77.51 6 |
| | ATOM | 4305 | CG | ASP C 129 | 28.304 | 56.729 | 57.486 | 1.00 | 78.34 6 |
| | ATOM | 4306 | OD1 | ASP C 129 | 29.328 | 56.051 | 57.770 | 1.00 | 78.50 8 |
| | ATOM | 4307 | OD2 | ASP C 129 | 27.132 | 56.377 | 57.803 | 1.00 | 77.23 8 |
| 50 | ATOM | 4308 | C | ASP C 129 | 26.114 | 58.634 | 56.235 | 1.00 | 78.98 6 |
| | ATOM | 4309 | O | ASP C 129 | 25.497 | 57.832 | 56.948 | 1.00 | 79.11 8 |
| | ATOM | 4310 | N | THR C 130 | 25.645 | 59.851 | 55.948 | 1.00 | 79.48 7 |
| | ATOM | 4311 | CA | THR C 130 | 24.365 | 60.250 | 56.521 | 1.00 | 80.50 6 |
| 55 | ATOM | 4312 | CB | THR C 130 | 24.447 | 60.229 | 58.077 | 1.00 | 83.19 6 |
| | ATOM | 4313 | OG1 | THR C 130 | 25.829 | 60.140 | 58.472 | 1.00 | 82.84 8 |
| | ATOM | 4314 | CG2 | THR C 130 | 23.618 | 59.035 | 58.670 | 1.00 | 83.96 6 |
| | ATOM | 4315 | C | THR C 130 | 23.705 | 61.566 | 56.146 | 1.00 | 79.50 6 |
| | ATOM | 4316 | O | THR C 130 | 24.362 | 62.536 | 55.760 | 1.00 | 78.71 8 |
| | ATOM | 4317 | N | GLU C 131 | 22.382 | 61.553 | 56.307 | 1.00 | 79.39 7 |
| 60 | ATOM | 4318 | CA | GLU C 131 | 21.486 | 62.700 | 56.114 | 1.00 | 79.61 6 |
| | ATOM | 4319 | CB | GLU C 131 | 21.981 | 63.893 | 56.961 | 1.00 | 82.70 6 |
| | ATOM | 4320 | CG | GLU C 131 | 21.680 | 63.772 | 58.471 | 1.00 | 85.13 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|----------|
| 5 | ATOM | 4321 | CD | GLU C 131 | 22.642 | 64.580 | 59.335 | 1.00 | 86.47 6 |
| | ATOM | 4322 | OE1 | GLU C 131 | 22.862 | 65.788 | 59.024 | 1.00 | 87.43 8 |
| | ATOM | 4323 | OE2 | GLU C 131 | 23.168 | 63.998 | 60.320 | 1.00 | 85.12 8 |
| | ATOM | 4324 | C | GLU C 131 | 21.207 | 63.185 | 54.715 | 1.00 | 77.86 6 |
| | ATOM | 4325 | O | GLU C 131 | 20.460 | 62.560 | 53.955 | 1.00 | 76.34 8 |
| 10 | ATOM | 4326 | N | SER C 132 | 21.771 | 64.355 | 54.428 | 1.00 | 76.46 7 |
| | ATOM | 4327 | CA | SER C 132 | 21.652 | 64.995 | 53.136 | 1.00 | 75.54 6 |
| | ATOM | 4328 | CB | SER C 132 | 21.941 | 66.495 | 53.290 | 1.00 | 76.21 6 |
| | ATOM | 4329 | OG | SER C 132 | 23.233 | 66.719 | 53.841 | 1.00 | 78.77 8 |
| | ATOM | 4330 | C | SER C 132 | 22.673 | 64.318 | 52.205 | 1.00 | 74.37 6 |
| 15 | ATOM | 4331 | O | SER C 132 | 22.799 | 64.675 | 51.026 | 1.00 | 74.56 8 |
| | ATOM | 4332 | N | GLY C 133 | 23.392 | 63.338 | 52.764 | 1.00 | 72.74 7 |
| | ATOM | 4333 | CA | GLY C 133 | 24.389 | 62.591 | 52.019 | 1.00 | 70.01 6 |
| | ATOM | 4334 | C | GLY C 133 | 25.435 | 63.449 | 51.337 | 1.00 | 68.98 6 |
| | ATOM | 4335 | O | GLY C 133 | 25.636 | 64.615 | 51.686 | 1.00 | 69.00 8 |
| 20 | ATOM | 4336 | N | ALA C 134 | 26.107 | 62.859 | 50.355 | 1.00 | 66.70 7 |
| | ATOM | 4337 | CA | ALA C 134 | 27.131 | 63.563 | 49.609 | 1.00 | 64.10 6 |
| | ATOM | 4338 | CB | ALA C 134 | 28.394 | 62.723 | 49.531 | 1.00 | 63.57 6 |
| | ATOM | 4339 | C | ALA C 134 | 26.641 | 63.899 | 48.212 | 1.00 | 62.41 6 |
| | ATOM | 4340 | O | ALA C 134 | 25.640 | 63.360 | 47.737 | 1.00 | 60.16 8 |
| 25 | ATOM | 4341 | N | THR C 135 | 27.347 | 64.826 | 47.573 | 1.00 | 62.33 7 |
| | ATOM | 4342 | CA | THR C 135 | 27.023 | 65.237 | 46.211 | 1.00 | 62.11 6 |
| | ATOM | 4343 | CB | THR C 135 | 26.431 | 66.642 | 46.166 | 1.00 | 61.79 6 |
| | ATOM | 4344 | OG1 | THR C 135 | 25.253 | 66.675 | 46.980 | 1.00 | 65.07 8 |
| | ATOM | 4345 | CG2 | THR C 135 | 26.057 | 67.007 | 44.746 | 1.00 | 60.95 6 |
| 30 | ATOM | 4346 | C | THR C 135 | 28.292 | 65.181 | 45.375 | 1.00 | 60.85 6 |
| | ATOM | 4347 | O | THR C 135 | 29.181 | 66.040 | 45.473 | 1.00 | 61.27 8 |
| | ATOM | 4348 | N | CYS C 136 | 28.368 | 64.128 | 44.574 | 1.00 | 58.77 7 |
| | ATOM | 4349 | CA | CYS C 136 | 29.499 | 63.891 | 43.712 | 1.00 | 56.58 6 |
| | ATOM | 4350 | C | CYS C 136 | 29.140 | 64.393 | 42.325 | 1.00 | 56.26 6 |
| 35 | ATOM | 4351 | O | CYS C 136 | 28.197 | 63.907 | 41.710 | 1.00 | 56.21 8 |
| | ATOM | 4352 | CB | CYS C 136 | 29.794 | 62.396 | 43.698 | 1.00 | 54.70 6 |
| | ATOM | 4353 | SG | CYS C 136 | 31.010 | 61.882 | 42.454 | 1.00 | 52.66 16 |
| | ATOM | 4354 | N | ARG C 137 | 29.874 | 65.386 | 41.843 | 1.00 | 55.40 7 |
| | ATOM | 4355 | CA | ARG C 137 | 29.605 | 65.938 | 40.520 | 1.00 | 55.61 6 |
| 40 | ATOM | 4356 | CB | ARG C 137 | 29.698 | 67.466 | 40.537 | 1.00 | 56.53 6 |
| | ATOM | 4357 | CG | ARG C 137 | 28.713 | 68.135 | 41.462 | 1.00 | 61.72 6 |
| | ATOM | 4358 | CD | ARG C 137 | 29.231 | 69.491 | 41.947 | 1.00 | 65.19 6 |
| | ATOM | 4359 | NE | ARG C 137 | 28.632 | 69.871 | 43.236 | 1.00 | 69.78 7 |
| | ATOM | 4360 | CZ | ARG C 137 | 27.352 | 70.221 | 43.412 | 1.00 | 71.88 6 |
| 45 | ATOM | 4361 | NH1 | ARG C 137 | 26.504 | 70.256 | 42.384 | 1.00 | 74.24 7 |
| | ATOM | 4362 | NH2 | ARG C 137 | 26.908 | 70.522 | 44.626 | 1.00 | 70.49 7 |
| | ATOM | 4363 | C | ARG C 137 | 30.604 | 65.392 | 39.522 | 1.00 | 55.23 6 |
| | ATOM | 4364 | O | ARG C 137 | 31.807 | 65.381 | 39.773 | 1.00 | 57.26 8 |
| | ATOM | 4365 | N | ILE C 138 | 30.095 | 64.948 | 38.385 | 1.00 | 52.01 7 |
| 50 | ATOM | 4366 | CA | ILE C 138 | 30.922 | 64.398 | 37.333 | 1.00 | 50.01 6 |
| | ATOM | 4367 | CB | ILE C 138 | 30.529 | 62.928 | 37.061 | 1.00 | 49.70 6 |
| | ATOM | 4368 | CG2 | ILE C 138 | 31.361 | 62.360 | 35.933 | 1.00 | 47.04 6 |
| | ATOM | 4369 | CG1 | ILE C 138 | 30.703 | 62.090 | 38.327 | 1.00 | 48.47 6 |
| | ATOM | 4370 | CD1 | ILE C 138 | 30.080 | 60.706 | 38.225 | 1.00 | 46.09 6 |
| 55 | ATOM | 4371 | C | ILE C 138 | 30.693 | 65.222 | 36.070 | 1.00 | 48.82 6 |
| | ATOM | 4372 | O | ILE C 138 | 29.571 | 65.322 | 35.597 | 1.00 | 46.40 8 |
| | ATOM | 4373 | N | LYS C 139 | 31.752 | 65.814 | 35.529 | 1.00 | 49.18 7 |
| | ATOM | 4374 | CA | LYS C 139 | 31.634 | 66.614 | 34.309 | 1.00 | 52.75 6 |
| | ATOM | 4375 | CB | LYS C 139 | 32.364 | 67.950 | 34.464 | 1.00 | 54.78 6 |
| 60 | ATOM | 4376 | CG | LYS C 139 | 31.952 | 68.737 | 35.697 | 1.00 | 59.35 6 |
| | ATOM | 4377 | CD | LYS C 139 | 32.477 | 70.168 | 35.669 | 1.00 | 60.96 6 |
| | ATOM | 4378 | CE | LYS C 139 | 31.780 | 71.019 | 34.594 | 1.00 | 62.06 6 |
| | ATOM | 4379 | NZ | LYS C 139 | 32.316 | 72.419 | 34.559 | 1.00 | 59.27 7 |
| | ATOM | 4380 | C | LYS C 139 | 32.218 | 65.886 | 33.106 | 1.00 | 52.07 6 |
| | ATOM | 4381 | O | LYS C 139 | 33.364 | 65.446 | 33.143 | 1.00 | 52.64 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 4382 | N | ILE | C | 140 | 31.441 | 65.761 | 32.036 | 1.00 | 51.29 | 7 |
| | ATOM | 4383 | CA | ILE | C | 140 | 31.938 | 65.091 | 30.842 | 1.00 | 50.15 | 6 |
| | ATOM | 4384 | CB | ILE | C | 140 | 31.404 | 63.613 | 30.769 | 1.00 | 51.22 | 6 |
| | ATOM | 4385 | CG2 | ILE | C | 140 | 31.536 | 62.955 | 32.134 | 1.00 | 52.05 | 6 |
| 5 | ATOM | 4386 | CG1 | ILE | C | 140 | 29.930 | 63.555 | 30.393 | 1.00 | 49.11 | 6 |
| | ATOM | 4387 | CD1 | ILE | C | 140 | 29.307 | 62.187 | 30.676 | 1.00 | 49.89 | 6 |
| | ATOM | 4388 | C | ILE | C | 140 | 31.624 | 65.861 | 29.560 | 1.00 | 47.99 | 6 |
| | ATOM | 4389 | O | ILE | C | 140 | 30.515 | 66.323 | 29.365 | 1.00 | 50.04 | 8 |
| | ATOM | 4390 | N | GLY | C | 141 | 32.620 | 66.025 | 28.701 | 1.00 | 46.57 | 7 |
| 10 | ATOM | 4391 | CA | GLY | C | 141 | 32.414 | 66.732 | 27.447 | 1.00 | 46.87 | 6 |
| | ATOM | 4392 | C | GLY | C | 141 | 33.453 | 66.323 | 26.416 | 1.00 | 46.66 | 6 |
| | ATOM | 4393 | O | GLY | C | 141 | 34.359 | 65.565 | 26.739 | 1.00 | 46.42 | 8 |
| | ATOM | 4394 | N | SER | C | 142 | 33.329 | 66.804 | 25.180 | 1.00 | 45.19 | 7 |
| | ATOM | 4395 | CA | SER | C | 142 | 34.303 | 66.474 | 24.140 | 1.00 | 41.98 | 6 |
| 15 | ATOM | 4396 | CB | SER | C | 142 | 33.974 | 67.165 | 22.828 | 1.00 | 40.96 | 6 |
| | ATOM | 4397 | OG | SER | C | 142 | 35.062 | 67.057 | 21.943 | 1.00 | 34.78 | 8 |
| | ATOM | 4398 | C | SER | C | 142 | 35.698 | 66.885 | 24.551 | 1.00 | 43.33 | 6 |
| | ATOM | 4399 | O | SER | C | 142 | 35.915 | 67.956 | 25.115 | 1.00 | 45.01 | 8 |
| | ATOM | 4400 | N | TRP | C | 143 | 36.655 | 66.028 | 24.256 | 1.00 | 43.12 | 7 |
| 20 | ATOM | 4401 | CA | TRP | C | 143 | 38.025 | 66.300 | 24.622 | 1.00 | 42.98 | 6 |
| | ATOM | 4402 | CB | TRP | C | 143 | 38.768 | 64.982 | 24.819 | 1.00 | 41.57 | 6 |
| | ATOM | 4403 | CG | TRP | C | 143 | 40.125 | 65.141 | 25.446 | 1.00 | 39.54 | 6 |
| | ATOM | 4404 | CD2 | TRP | C | 143 | 40.394 | 65.420 | 26.820 | 1.00 | 36.50 | 6 |
| | ATOM | 4405 | CE2 | TRP | C | 143 | 41.795 | 65.481 | 26.967 | 1.00 | 35.30 | 6 |
| 25 | ATOM | 4406 | CE3 | TRP | C | 143 | 39.584 | 65.625 | 27.943 | 1.00 | 36.55 | 6 |
| | ATOM | 4407 | CD1 | TRP | C | 143 | 41.345 | 65.048 | 24.829 | 1.00 | 38.96 | 6 |
| | ATOM | 4408 | NE1 | TRP | C | 143 | 42.353 | 65.251 | 25.738 | 1.00 | 35.00 | 7 |
| | ATOM | 4409 | CZ2 | TRP | C | 143 | 42.400 | 65.736 | 28.192 | 1.00 | 34.47 | 6 |
| | ATOM | 4410 | CZ3 | TRP | C | 143 | 40.185 | 65.878 | 29.153 | 1.00 | 35.28 | 6 |
| 30 | ATOM | 4411 | CH2 | TRP | C | 143 | 41.580 | 65.931 | 29.271 | 1.00 | 35.16 | 6 |
| | ATOM | 4412 | C | TRP | C | 143 | 38.767 | 67.159 | 23.605 | 1.00 | 43.69 | 6 |
| | ATOM | 4413 | O | TRP | C | 143 | 39.657 | 67.915 | 23.962 | 1.00 | 46.65 | 8 |
| | ATOM | 4414 | N | THR | C | 144 | 38.402 | 67.065 | 22.338 | 1.00 | 42.21 | 7 |
| | ATOM | 4415 | CA | THR | C | 144 | 39.107 | 67.834 | 21.333 | 1.00 | 40.90 | 6 |
| 35 | ATOM | 4416 | CB | THR | C | 144 | 39.839 | 66.901 | 20.372 | 1.00 | 40.06 | 6 |
| | ATOM | 4417 | OG1 | THR | C | 144 | 38.907 | 65.976 | 19.798 | 1.00 | 40.17 | 8 |
| | ATOM | 4418 | CG2 | THR | C | 144 | 40.916 | 66.144 | 21.106 | 1.00 | 38.34 | 6 |
| | ATOM | 4419 | C | THR | C | 144 | 38.252 | 68.795 | 20.520 | 1.00 | 43.03 | 6 |
| | ATOM | 4420 | O | THR | C | 144 | 38.786 | 69.631 | 19.795 | 1.00 | 43.02 | 8 |
| 40 | ATOM | 4421 | N | HIS | C | 145 | 36.934 | 68.687 | 20.635 | 1.00 | 42.41 | 7 |
| | ATOM | 4422 | CA | HIS | C | 145 | 36.065 | 69.571 | 19.885 | 1.00 | 45.42 | 6 |
| | ATOM | 4423 | CB | HIS | C | 145 | 34.994 | 68.772 | 19.144 | 1.00 | 48.25 | 6 |
| | ATOM | 4424 | CG | HIS | C | 145 | 35.533 | 67.873 | 18.071 | 1.00 | 49.32 | 6 |
| | ATOM | 4425 | CD2 | HIS | C | 145 | 36.052 | 68.154 | 16.853 | 1.00 | 47.20 | 6 |
| 45 | ATOM | 4426 | ND1 | HIS | C | 145 | 35.572 | 66.500 | 18.197 | 1.00 | 47.13 | 7 |
| | ATOM | 4427 | CE1 | HIS | C | 145 | 36.091 | 65.976 | 17.103 | 1.00 | 47.99 | 6 |
| | ATOM | 4428 | NE2 | HIS | C | 145 | 36.391 | 66.958 | 16.272 | 1.00 | 48.34 | 7 |
| | ATOM | 4429 | C | HIS | C | 145 | 35.394 | 70.627 | 20.754 | 1.00 | 48.71 | 6 |
| | ATOM | 4430 | O | HIS | C | 145 | 34.738 | 70.325 | 21.746 | 1.00 | 47.60 | 8 |
| 50 | ATOM | 4431 | N | HIS | C | 146 | 35.562 | 71.883 | 20.363 | 1.00 | 52.53 | 7 |
| | ATOM | 4432 | CA | HIS | C | 146 | 34.972 | 72.993 | 21.094 | 1.00 | 53.12 | 6 |
| | ATOM | 4433 | CB | HIS | C | 146 | 35.777 | 74.261 | 20.840 | 1.00 | 50.98 | 6 |
| | ATOM | 4434 | CG | HIS | C | 146 | 35.931 | 74.586 | 19.390 | 1.00 | 48.89 | 6 |
| | ATOM | 4435 | CD2 | HIS | C | 146 | 35.013 | 74.755 | 18.409 | 1.00 | 47.83 | 6 |
| 55 | ATOM | 4436 | ND1 | HIS | C | 146 | 37.161 | 74.776 | 18.801 | 1.00 | 48.82 | 7 |
| | ATOM | 4437 | CE1 | HIS | C | 146 | 36.993 | 75.049 | 17.519 | 1.00 | 48.32 | 6 |
| | ATOM | 4438 | NE2 | HIS | C | 146 | 35.699 | 75.043 | 17.257 | 1.00 | 46.12 | 7 |
| | ATOM | 4439 | C | HIS | C | 146 | 33.524 | 73.188 | 20.664 | 1.00 | 54.19 | 6 |
| | ATOM | 4440 | O | HIS | C | 146 | 33.047 | 72.531 | 19.736 | 1.00 | 54.21 | 8 |
| 60 | ATOM | 4441 | N | SER | C | 147 | 32.847 | 74.112 | 21.341 | 1.00 | 56.30 | 7 |
| | ATOM | 4442 | CA | SER | C | 147 | 31.437 | 74.418 | 21.115 | 1.00 | 57.23 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 4443 | CB | SER C 147 | 31.055 | 75.610 | 21.978 | 1.00 | 57.36 | 6 | |
| | ATOM | 4444 | OG | SER C 147 | 32.017 | 76.635 | 21.828 | 1.00 | 59.18 | 8 | |
| | ATOM | 4445 | C | SER C 147 | 30.972 | 74.660 | 19.682 | 1.00 | 57.72 | 6 | |
| | ATOM | 4446 | O | SER C 147 | 29.790 | 74.484 | 19.375 | 1.00 | 57.25 | 8 | |
| | ATOM | 4447 | N | ARG C 148 | 31.885 | 75.065 | 18.809 | 1.00 | 58.23 | 7 | |
| 10 | ATOM | 4448 | CA | ARG C 148 | 31.517 | 75.336 | 17.424 | 1.00 | 60.12 | 6 | |
| | ATOM | 4449 | CB | ARG C 148 | 32.555 | 76.264 | 16.777 | 1.00 | 63.75 | 6 | |
| | ATOM | 4450 | CG | ARG C 148 | 32.799 | 77.567 | 17.549 | 1.00 | 70.83 | 6 | |
| | ATOM | 4451 | CD | ARG C 148 | 33.950 | 78.393 | 16.946 | 1.00 | 77.31 | 6 | |
| | ATOM | 4452 | NE | ARG C 148 | 34.422 | 79.453 | 17.852 | 1.00 | 84.18 | 7 | |
| 15 | ATOM | 4453 | CZ | ARG C 148 | 33.696 | 80.506 | 18.245 | 1.00 | 86.23 | 6 | |
| | ATOM | 4454 | NH1 | ARG C 148 | 32.447 | 80.661 | 17.818 | 1.00 | 87.64 | 7 | |
| | ATOM | 4455 | NH2 | ARG C 148 | 34.213 | 81.408 | 19.072 | 1.00 | 86.26 | 7 | |
| | ATOM | 4456 | C | ARG C 148 | 31.390 | 74.051 | 16.601 | 1.00 | 59.83 | 6 | |
| | ATOM | 4457 | O | ARG C 148 | 30.786 | 74.053 | 15.519 | 1.00 | 60.30 | 8 | |
| 20 | ATOM | 4458 | N | GLU C 149 | 31.954 | 72.959 | 17.121 | 1.00 | 57.69 | 7 | |
| | ATOM | 4459 | CA | GLU C 149 | 31.937 | 71.677 | 16.425 | 1.00 | 54.67 | 6 | |
| | ATOM | 4460 | CB | GLU C 149 | 33.364 | 71.132 | 16.321 | 1.00 | 52.47 | 6 | |
| | ATOM | 4461 | CG | GLU C 149 | 34.395 | 72.228 | 16.050 | 1.00 | 52.11 | 6 | |
| | ATOM | 4462 | CD | GLU C 149 | 35.824 | 71.718 | 15.896 | 1.00 | 50.20 | 6 | |
| 25 | ATOM | 4463 | OE1 | GLU C 149 | 36.246 | 70.852 | 16.678 | 1.00 | 49.43 | 8 | |
| | ATOM | 4464 | OE2 | GLU C 149 | 36.537 | 72.203 | 15.004 | 1.00 | 47.62 | 8 | |
| | ATOM | 4465 | C | GLU C 149 | 31.043 | 70.698 | 17.162 | 1.00 | 53.64 | 6 | |
| | ATOM | 4466 | O | GLU C 149 | 30.252 | 69.985 | 16.552 | 1.00 | 53.16 | 8 | |
| | ATOM | 4467 | N | ILE C 150 | 31.172 | 70.667 | 18.479 | 1.00 | 52.16 | 7 | |
| 30 | ATOM | 4468 | CA | ILE C 150 | 30.353 | 69.795 | 19.289 | 1.00 | 51.98 | 6 | |
| | ATOM | 4469 | CB | ILE C 150 | 31.157 | 68.612 | 19.883 | 1.00 | 53.49 | 6 | |
| | ATOM | 4470 | CG2 | ILE C 150 | 30.361 | 67.954 | 21.019 | 1.00 | 52.00 | 6 | |
| | ATOM | 4471 | CG1 | ILE C 150 | 31.450 | 67.571 | 18.800 | 1.00 | 53.48 | 6 | |
| | ATOM | 4472 | CD1 | ILE C 150 | 32.235 | 66.383 | 19.299 | 1.00 | 50.44 | 6 | |
| 35 | ATOM | 4473 | C | ILE C 150 | 29.750 | 70.565 | 20.446 | 1.00 | 53.26 | 6 | |
| | ATOM | 4474 | O | ILE C 150 | 30.410 | 71.389 | 21.095 | 1.00 | 51.01 | 8 | |
| | ATOM | 4475 | N | SER C 151 | 28.479 | 70.280 | 20.694 | 1.00 | 54.99 | 7 | |
| | ATOM | 4476 | CA | SER C 151 | 27.749 | 70.887 | 21.797 | 1.00 | 56.94 | 6 | |
| | ATOM | 4477 | CB | SER C 151 | 26.693 | 71.873 | 21.280 | 1.00 | 54.85 | 6 | |
| 40 | ATOM | 4478 | OG | SER C 151 | 25.665 | 71.221 | 20.557 | 1.00 | 55.92 | 8 | |
| | ATOM | 4479 | C | SER C 151 | 27.084 | 69.717 | 22.516 | 1.00 | 59.00 | 6 | |
| | ATOM | 4480 | O | SER C 151 | 26.536 | 68.820 | 21.871 | 1.00 | 60.03 | 8 | |
| | ATOM | 4481 | N | VAL C 152 | 27.172 | 69.705 | 23.844 | 1.00 | 60.32 | 7 | |
| | ATOM | 4482 | CA | VAL C 152 | 26.569 | 68.651 | 24.655 | 1.00 | 61.16 | 6 | |
| 45 | ATOM | 4483 | CB | VAL C 152 | 27.564 | 68.096 | 25.694 | 1.00 | 60.14 | 6 | |
| | ATOM | 4484 | CG1 | VAL C 152 | 28.858 | 67.723 | 25.009 | 1.00 | 61.98 | 6 | |
| | ATOM | 4485 | CG2 | VAL C 152 | 27.817 | 69.110 | 26.775 | 1.00 | 61.23 | 6 | |
| | ATOM | 4486 | C | VAL C 152 | 25.373 | 69.237 | 25.391 | 1.00 | 62.82 | 6 | |
| | ATOM | 4487 | O | VAL C 152 | 25.379 | 70.409 | 25.758 | 1.00 | 63.73 | 8 | |
| 50 | ATOM | 4488 | N | ASP C 153 | 24.349 | 68.425 | 25.614 | 1.00 | 65.81 | 7 | |
| | ATOM | 4489 | CA | ASP C 153 | 23.147 | 68.887 | 26.293 | 1.00 | 67.23 | 6 | |
| | ATOM | 4490 | CB | ASP C 153 | 22.150 | 69.377 | 25.249 | 1.00 | 69.19 | 6 | |
| | ATOM | 4491 | CG | ASP C 153 | 22.748 | 70.425 | 24.320 | 1.00 | 72.38 | 6 | |
| | ATOM | 4492 | OD1 | ASP C 153 | 22.786 | 71.614 | 24.718 | 1.00 | 72.90 | 8 | |
| 55 | ATOM | 4493 | OD2 | ASP C 153 | 23.193 | 70.060 | 23.201 | 1.00 | 75.01 | 8 | |
| | ATOM | 4494 | C | ASP C 153 | 22.505 | 67.776 | 27.120 | 1.00 | 69.10 | 6 | |
| | ATOM | 4495 | O | ASP C 153 | 22.504 | 66.612 | 26.717 | 1.00 | 68.47 | 8 | |
| | ATOM | 4496 | N | PRO C 154 | 21.970 | 68.115 | 28.304 | 1.00 | 70.49 | 7 | |
| | ATOM | 4497 | CD | PRO C 154 | 22.282 | 69.309 | 29.094 | 1.00 | 69.97 | 6 | |
| 60 | ATOM | 4498 | CA | PRO C 154 | 21.325 | 67.098 | 29.147 | 1.00 | 73.18 | 6 | |
| | ATOM | 4499 | CB | PRO C 154 | 21.148 | 67.814 | 30.477 | 1.00 | 70.84 | 6 | |
| | ATOM | 4500 | CG | PRO C 154 | 22.300 | 68.745 | 30.493 | 1.00 | 71.35 | 6 | |
| | ATOM | 4501 | C | PRO C 154 | 19.985 | 66.669 | 28.522 | 1.00 | 77.25 | 6 | |
| | ATOM | 4502 | O | PRO C 154 | 19.591 | 67.183 | 27.462 | 1.00 | 77.76 | 8 | |
| | ATOM | 4503 | N | THR C 155 | 19.279 | 65.744 | 29.175 | 1.00 | 80.57 | 7 | |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|---|
| | ATOM | 4504 | CA | THR | C | 155 | 18.010 | 65.253 | 28.633 | 1.00 | 83.84 | 6 |
| | ATOM | 4505 | CB | THR | C | 155 | 18.244 | 63.932 | 27.837 | 1.00 | 83.53 | 6 |
| | ATOM | 4506 | OG1 | THR | C | 155 | 18.609 | 62.882 | 28.744 | 1.00 | 83.26 | 8 |
| | ATOM | 4507 | CG2 | THR | C | 155 | 19.361 | 64.105 | 26.823 | 1.00 | 83.08 | 6 |
| 5 | ATOM | 4508 | C | THR | C | 155 | 16.897 | 65.001 | 29.678 | 1.00 | 87.74 | 6 |
| | ATOM | 4509 | O | THR | C | 155 | 16.826 | 65.677 | 30.715 | 1.00 | 87.94 | 8 |
| | ATOM | 4510 | N | THR | C | 156 | 16.042 | 64.012 | 29.370 | 1.00 | 91.72 | 7 |
| | ATOM | 4511 | CA | THR | C | 156 | 14.882 | 63.577 | 30.180 | 1.00 | 93.73 | 6 |
| 10 | ATOM | 4512 | CB | THR | C | 156 | 14.501 | 62.092 | 29.877 | 1.00 | 93.94 | 6 |
| | ATOM | 4513 | OG1 | THR | C | 156 | 14.249 | 61.933 | 28.470 | 1.00 | 93.93 | 8 |
| | ATOM | 4514 | CG2 | THR | C | 156 | 13.253 | 61.681 | 30.696 | 1.00 | 93.29 | 6 |
| | ATOM | 4515 | C | THR | C | 156 | 15.042 | 63.695 | 31.693 | 1.00 | 95.32 | 6 |
| | ATOM | 4516 | O | THR | C | 156 | 15.626 | 62.817 | 32.347 | 1.00 | 95.61 | 8 |
| | ATOM | 4517 | N | GLU | C | 157 | 14.490 | 64.767 | 32.246 | 1.00 | 97.07 | 7 |
| 15 | ATOM | 4518 | CA | GLU | C | 157 | 14.578 | 65.011 | 33.679 | 1.00 | 98.94 | 6 |
| | ATOM | 4519 | CB | GLU | C | 157 | 14.487 | 66.514 | 33.942 | 1.00 | 100.27 | 6 |
| | ATOM | 4520 | CG | GLU | C | 157 | 15.282 | 67.359 | 32.950 | 1.00 | 102.55 | 6 |
| | ATOM | 4521 | CD | GLU | C | 157 | 15.113 | 68.852 | 33.214 | 1.00 | 104.54 | 6 |
| 20 | ATOM | 4522 | OE1 | GLU | C | 157 | 13.943 | 69.322 | 33.312 | 1.00 | 105.88 | 8 |
| | ATOM | 4523 | OE2 | GLU | C | 157 | 16.150 | 69.555 | 33.327 | 1.00 | 104.90 | 8 |
| | ATOM | 4524 | C | GLU | C | 157 | 13.475 | 64.290 | 34.465 | 1.00 | 99.30 | 6 |
| | ATOM | 4525 | O | GLU | C | 157 | 13.452 | 64.337 | 35.706 | 1.00 | 99.77 | 8 |
| | ATOM | 4526 | N | ASN | C | 158 | 12.557 | 63.639 | 33.751 | 1.00 | 99.15 | 7 |
| 25 | ATOM | 4527 | CA | ASN | C | 158 | 11.457 | 62.919 | 34.404 | 1.00 | 98.32 | 6 |
| | ATOM | 4528 | CB | ASN | C | 158 | 10.382 | 62.541 | 33.374 | 1.00 | 100.43 | 6 |
| | ATOM | 4529 | CG | ASN | C | 158 | 9.902 | 63.736 | 32.555 | 1.00 | 101.38 | 6 |
| | ATOM | 4530 | OD1 | ASN | C | 158 | 9.423 | 64.738 | 33.112 | 1.00 | 101.96 | 8 |
| | ATOM | 4531 | ND2 | ASN | C | 158 | 10.026 | 63.636 | 31.224 | 1.00 | 101.40 | 7 |
| 30 | ATOM | 4532 | C | ASN | C | 158 | 11.991 | 61.638 | 35.064 | 1.00 | 96.64 | 6 |
| | ATOM | 4533 | O | ASN | C | 158 | 12.380 | 61.643 | 36.239 | 1.00 | 96.33 | 8 |
| | ATOM | 4534 | N | SER | C | 159 | 11.992 | 60.558 | 34.283 | 1.00 | 93.61 | 7 |
| | ATOM | 4535 | CA | SER | C | 159 | 12.466 | 59.237 | 34.690 | 1.00 | 90.35 | 6 |
| | ATOM | 4536 | CB | SER | C | 159 | 13.541 | 58.788 | 33.690 | 1.00 | 90.84 | 6 |
| | ATOM | 4537 | OG | SER | C | 159 | 14.367 | 59.898 | 33.320 | 1.00 | 90.44 | 8 |
| 35 | ATOM | 4538 | C | SER | C | 159 | 13.005 | 59.167 | 36.123 | 1.00 | 88.15 | 6 |
| | ATOM | 4539 | O | SER | C | 159 | 13.942 | 59.894 | 36.481 | 1.00 | 88.99 | 8 |
| | ATOM | 4540 | N | ASP | C | 160 | 12.414 | 58.302 | 36.945 | 1.00 | 84.53 | 7 |
| | ATOM | 4541 | CA | ASP | C | 160 | 12.863 | 58.152 | 38.330 | 1.00 | 80.47 | 6 |
| 40 | ATOM | 4542 | CB | ASP | C | 160 | 12.232 | 56.921 | 38.985 | 1.00 | 80.26 | 6 |
| | ATOM | 4543 | CG | ASP | C | 160 | 12.760 | 56.683 | 40.398 | 1.00 | 82.12 | 6 |
| | ATOM | 4544 | OD1 | ASP | C | 160 | 12.658 | 55.536 | 40.890 | 1.00 | 82.78 | 8 |
| | ATOM | 4545 | OD2 | ASP | C | 160 | 13.277 | 57.644 | 41.023 | 1.00 | 82.17 | 8 |
| | ATOM | 4546 | C | ASP | C | 160 | 14.380 | 57.978 | 38.340 | 1.00 | 77.39 | 6 |
| | ATOM | 4547 | O | ASP | C | 160 | 14.892 | 57.009 | 37.768 | 1.00 | 75.75 | 8 |
| 45 | ATOM | 4548 | N | ASP | C | 161 | 15.080 | 58.910 | 38.992 | 1.00 | 73.66 | 7 |
| | ATOM | 4549 | CA | ASP | C | 161 | 16.529 | 58.864 | 39.072 | 1.00 | 71.77 | 6 |
| | ATOM | 4550 | CB | ASP | C | 161 | 17.060 | 59.934 | 40.028 | 1.00 | 71.93 | 6 |
| | ATOM | 4551 | CG | ASP | C | 161 | 16.943 | 61.330 | 39.461 | 1.00 | 72.28 | 6 |
| 50 | ATOM | 4552 | OD1 | ASP | C | 161 | 17.115 | 61.486 | 38.230 | 1.00 | 71.71 | 8 |
| | ATOM | 4553 | OD2 | ASP | C | 161 | 16.695 | 62.270 | 40.246 | 1.00 | 74.13 | 8 |
| | ATOM | 4554 | C | ASP | C | 161 | 17.118 | 57.515 | 39.479 | 1.00 | 70.97 | 6 |
| | ATOM | 4555 | O | ASP | C | 161 | 18.296 | 57.251 | 39.222 | 1.00 | 73.00 | 8 |
| | ATOM | 4556 | N | SER | C | 162 | 16.335 | 56.649 | 40.105 | 1.00 | 68.54 | 7 |
| | ATOM | 4557 | CA | SER | C | 162 | 16.899 | 55.366 | 40.496 | 1.00 | 66.65 | 6 |
| 55 | ATOM | 4558 | CB | SER | C | 162 | 17.085 | 55.308 | 42.020 | 1.00 | 66.09 | 6 |
| | ATOM | 4559 | OG | SER | C | 162 | 15.845 | 55.352 | 42.698 | 1.00 | 66.84 | 8 |
| | ATOM | 4560 | C | SER | C | 162 | 16.064 | 54.194 | 40.019 | 1.00 | 65.29 | 6 |
| | ATOM | 4561 | O | SER | C | 162 | 16.042 | 53.147 | 40.646 | 1.00 | 65.08 | 8 |
| 60 | ATOM | 4562 | N | GLU | C | 163 | 15.393 | 54.357 | 38.892 | 1.00 | 64.69 | 7 |
| | ATOM | 4563 | CA | GLU | C | 163 | 14.571 | 53.270 | 38.398 | 1.00 | 66.58 | 6 |
| | ATOM | 4564 | CB | GLU | C | 163 | 13.543 | 53.784 | 37.372 | 1.00 | 68.86 | 6 |

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|----|------|------|-----|-----|------|-----|--------|--------|--------|--------------|
| | ATOM | 4565 | CG | GLU | C | 163 | 14.029 | 53.942 | 35.951 | 1.00 70.35 6 |
| | ATOM | 4566 | CD | GLU | C | 163 | 12.886 | 54.261 | 35.000 | 1.00 73.03 6 |
| | ATOM | 4567 | OE1 | GLU | C | 163 | 12.345 | 55.390 | 35.065 | 1.00 75.39 8 |
| | ATOM | 4568 | OE2 | GLU | C | 163 | 12.517 | 53.378 | 34.193 | 1.00 72.63 8 |
| 5 | ATOM | 4569 | C | GLU | C | 163 | 15.416 | 52.145 | 37.808 | 1.00 65.46 6 |
| | ATOM | 4570 | O | GLU | C | 163 | 14.902 | 51.071 | 37.481 | 1.00 64.98 8 |
| | ATOM | 4571 | N | TYR | C | 164 | 16.718 | 52.392 | 37.675 | 1.00 65.54 7 |
| | ATOM | 4572 | CA | TYR | C | 164 | 17.647 | 51.389 | 37.143 | 1.00 63.20 6 |
| | ATOM | 4573 | CB | TYR | C | 164 | 18.353 | 51.894 | 35.884 | 1.00 63.41 6 |
| 10 | ATOM | 4574 | CG | TYR | C | 164 | 17.433 | 52.101 | 34.716 | 1.00 65.49 6 |
| | ATOM | 4575 | CD1 | TYR | C | 164 | 17.299 | 53.355 | 34.119 | 1.00 66.61 6 |
| | ATOM | 4576 | CE1 | TYR | C | 164 | 16.429 | 53.555 | 33.046 | 1.00 68.54 6 |
| | ATOM | 4577 | CD2 | TYR | C | 164 | 16.676 | 51.046 | 34.216 | 1.00 68.25 6 |
| | ATOM | 4578 | CE2 | TYR | C | 164 | 15.797 | 51.230 | 33.144 | 1.00 70.31 6 |
| 15 | ATOM | 4579 | CZ | TYR | C | 164 | 15.680 | 52.484 | 32.562 | 1.00 70.26 6 |
| | ATOM | 4580 | OH | TYR | C | 164 | 14.832 | 52.655 | 31.482 | 1.00 74.21 8 |
| | ATOM | 4581 | C | TYR | C | 164 | 18.690 | 51.066 | 38.184 | 1.00 61.13 6 |
| | ATOM | 4582 | O | TYR | C | 164 | 19.480 | 50.147 | 38.003 | 1.00 60.53 8 |
| | ATOM | 4583 | N | PHE | C | 165 | 18.687 | 51.824 | 39.279 | 1.00 59.92 7 |
| 20 | ATOM | 4584 | CA | PHE | C | 165 | 19.657 | 51.622 | 40.347 | 1.00 58.58 6 |
| | ATOM | 4585 | CB | PHE | C | 165 | 19.497 | 52.690 | 41.425 | 1.00 56.39 6 |
| | ATOM | 4586 | CG | PHE | C | 165 | 20.717 | 52.856 | 42.288 | 1.00 55.60 6 |
| | ATOM | 4587 | CD1 | PHE | C | 165 | 21.904 | 53.336 | 41.742 | 1.00 53.27 6 |
| | ATOM | 4588 | CD2 | PHE | C | 165 | 20.692 | 52.497 | 43.629 | 1.00 54.20 6 |
| 25 | ATOM | 4589 | CE1 | PHE | C | 165 | 23.049 | 53.451 | 42.513 | 1.00 53.30 6 |
| | ATOM | 4590 | CE2 | PHE | C | 165 | 21.835 | 52.607 | 44.414 | 1.00 54.70 6 |
| | ATOM | 4591 | CZ | PHE | C | 165 | 23.018 | 53.085 | 43.854 | 1.00 54.90 6 |
| | ATOM | 4592 | C | PHE | C | 165 | 19.528 | 50.250 | 40.974 | 1.00 58.64 6 |
| | ATOM | 4593 | O | PHE | C | 165 | 18.422 | 49.749 | 41.153 | 1.00 60.35 8 |
| 30 | ATOM | 4594 | N | SER | C | 166 | 20.655 | 49.631 | 41.298 | 1.00 58.50 7 |
| | ATOM | 4595 | CA | SER | C | 166 | 20.614 | 48.309 | 41.900 | 1.00 58.50 6 |
| | ATOM | 4596 | CB | SER | C | 166 | 22.013 | 47.703 | 41.996 | 1.00 58.83 6 |
| | ATOM | 4597 | OG | SER | C | 166 | 21.957 | 46.391 | 42.542 | 1.00 61.34 8 |
| | ATOM | 4598 | C | SER | C | 166 | 20.050 | 48.473 | 43.286 | 1.00 58.49 6 |
| 35 | ATOM | 4599 | O | SER | C | 166 | 20.346 | 49.454 | 43.964 | 1.00 58.40 8 |
| | ATOM | 4600 | N | GLN | C | 167 | 19.249 | 47.503 | 43.706 | 1.00 57.37 7 |
| | ATOM | 4601 | CA | GLN | C | 167 | 18.631 | 47.545 | 45.020 | 1.00 57.17 6 |
| | ATOM | 4602 | CB | GLN | C | 167 | 17.317 | 46.766 | 44.994 | 1.00 59.70 6 |
| | ATOM | 4603 | CG | GLN | C | 167 | 17.467 | 45.351 | 44.490 | 1.00 62.90 6 |
| 40 | ATOM | 4604 | CD | GLN | C | 167 | 16.136 | 44.696 | 44.164 | 1.00 67.19 6 |
| | ATOM | 4605 | OE1 | GLN | C | 167 | 15.284 | 44.519 | 45.048 | 1.00 68.37 8 |
| | ATOM | 4606 | NE2 | GLN | C | 167 | 15.940 | 44.334 | 42.884 | 1.00 66.77 7 |
| | ATOM | 4607 | C | GLN | C | 167 | 19.548 | 46.975 | 46.085 | 1.00 55.30 6 |
| | ATOM | 4608 | O | GLN | C | 167 | 19.373 | 47.235 | 47.271 | 1.00 53.36 8 |
| 45 | ATOM | 4609 | N | TYR | C | 168 | 20.541 | 46.211 | 45.659 | 1.00 55.00 7 |
| | ATOM | 4610 | CA | TYR | C | 168 | 21.455 | 45.601 | 46.609 | 1.00 55.48 6 |
| | ATOM | 4611 | CB | TYR | C | 168 | 21.845 | 44.214 | 46.114 | 1.00 55.25 6 |
| | ATOM | 4612 | CG | TYR | C | 168 | 20.630 | 43.413 | 45.714 | 1.00 56.93 6 |
| | ATOM | 4613 | CD1 | TYR | C | 168 | 20.242 | 43.315 | 44.378 | 1.00 56.29 6 |
| 50 | ATOM | 4614 | CE1 | TYR | C | 168 | 19.087 | 42.640 | 44.016 | 1.00 56.50 6 |
| | ATOM | 4615 | CD2 | TYR | C | 168 | 19.825 | 42.809 | 46.680 | 1.00 57.12 6 |
| | ATOM | 4616 | CE2 | TYR | C | 168 | 18.664 | 42.133 | 46.332 | 1.00 56.97 6 |
| | ATOM | 4617 | CZ | TYR | C | 168 | 18.300 | 42.054 | 44.997 | 1.00 58.82 6 |
| | ATOM | 4618 | OH | TYR | C | 168 | 17.133 | 41.408 | 44.640 | 1.00 61.29 8 |
| 55 | ATOM | 4619 | C | TYR | C | 168 | 22.692 | 46.431 | 46.919 | 1.00 55.31 6 |
| | ATOM | 4620 | O | TYR | C | 168 | 23.582 | 45.987 | 47.637 | 1.00 53.34 8 |
| | ATOM | 4621 | N | SER | C | 169 | 22.733 | 47.646 | 46.384 | 1.00 56.64 7 |
| | ATOM | 4622 | CA | SER | C | 169 | 23.851 | 48.553 | 46.620 | 1.00 58.01 6 |
| | ATOM | 4623 | CB | SER | C | 169 | 23.731 | 49.786 | 45.720 | 1.00 58.39 6 |
| 60 | ATOM | 4624 | OG | SER | C | 169 | 24.745 | 50.727 | 46.017 | 1.00 57.32 8 |
| | ATOM | 4625 | C | SER | C | 169 | 23.860 | 49.001 | 48.076 | 1.00 60.12 6 |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 4626 | O SER C 169 | 22.803 | 49.148 | 48.699 | 1.00 | 60.78 | 8 |
| | ATOM | 4627 | N ARG C 170 | 25.052 | 49.215 | 48.621 | 1.00 | 59.44 | 7 |
| | ATOM | 4628 | CA ARG C 170 | 25.174 | 49.662 | 49.998 | 1.00 | 58.39 | 6 |
| | ATOM | 4629 | CB ARG C 170 | 26.636 | 49.602 | 50.438 | 1.00 | 59.12 | 6 |
| | ATOM | 4630 | CG ARG C 170 | 26.999 | 48.350 | 51.195 | 1.00 | 61.61 | 6 |
| 10 | ATOM | 4631 | CD ARG C 170 | 28.466 | 47.972 | 51.024 | 1.00 | 64.86 | 6 |
| | ATOM | 4632 | NE ARG C 170 | 29.418 | 49.012 | 51.424 | 1.00 | 66.40 | 7 |
| | ATOM | 4633 | CZ ARG C 170 | 30.317 | 49.556 | 50.597 | 1.00 | 68.28 | 6 |
| | ATOM | 4634 | NH1 ARG C 170 | 30.384 | 49.165 | 49.326 | 1.00 | 66.23 | 7 |
| | ATOM | 4635 | NH2 ARG C 170 | 31.166 | 50.480 | 51.039 | 1.00 | 68.62 | 7 |
| 15 | ATOM | 4636 | C ARG C 170 | 24.668 | 51.102 | 50.109 | 1.00 | 59.25 | 6 |
| | ATOM | 4637 | O ARG C 170 | 24.416 | 51.609 | 51.215 | 1.00 | 59.99 | 8 |
| | ATOM | 4638 | N PHE C 171 | 24.498 | 51.759 | 48.968 | 1.00 | 57.06 | 7 |
| | ATOM | 4639 | CA PHE C 171 | 24.063 | 53.146 | 48.982 | 1.00 | 56.45 | 6 |
| | ATOM | 4640 | CB PHE C 171 | 25.131 | 54.016 | 48.324 | 1.00 | 55.23 | 6 |
| 20 | ATOM | 4641 | CG PHE C 171 | 26.521 | 53.719 | 48.814 | 1.00 | 54.51 | 6 |
| | ATOM | 4642 | CD1 PHE C 171 | 27.189 | 52.568 | 48.400 | 1.00 | 55.98 | 6 |
| | ATOM | 4643 | CD2 PHE C 171 | 27.145 | 54.559 | 49.724 | 1.00 | 53.29 | 6 |
| | ATOM | 4644 | CE1 PHE C 171 | 28.463 | 52.257 | 48.890 | 1.00 | 55.09 | 6 |
| | ATOM | 4645 | CE2 PHE C 171 | 28.412 | 54.258 | 50.218 | 1.00 | 54.24 | 6 |
| 25 | ATOM | 4646 | CZ PHE C 171 | 29.074 | 53.102 | 49.799 | 1.00 | 54.89 | 6 |
| | ATOM | 4647 | C PHE C 171 | 22.732 | 53.346 | 48.311 | 1.00 | 55.77 | 6 |
| | ATOM | 4648 | O PHE C 171 | 22.164 | 52.406 | 47.761 | 1.00 | 55.57 | 8 |
| | ATOM | 4649 | N GLU C 172 | 22.228 | 54.569 | 48.376 | 1.00 | 55.26 | 7 |
| | ATOM | 4650 | CA GLU C 172 | 20.947 | 54.877 | 47.760 | 1.00 | 58.65 | 6 |
| 30 | ATOM | 4651 | CB GLU C 172 | 19.806 | 54.769 | 48.789 | 1.00 | 60.96 | 6 |
| | ATOM | 4652 | CG GLU C 172 | 19.891 | 55.739 | 49.981 | 1.00 | 64.19 | 6 |
| | ATOM | 4653 | CD GLU C 172 | 18.753 | 55.551 | 50.992 | 1.00 | 64.82 | 6 |
| | ATOM | 4654 | OE1 GLU C 172 | 17.626 | 55.236 | 50.557 | 1.00 | 65.38 | 8 |
| | ATOM | 4655 | OE2 GLU C 172 | 18.976 | 55.734 | 52.216 | 1.00 | 64.87 | 8 |
| 35 | ATOM | 4656 | C GLU C 172 | 21.014 | 56.279 | 47.162 | 1.00 | 59.71 | 6 |
| | ATOM | 4657 | O GLU C 172 | 21.815 | 57.116 | 47.600 | 1.00 | 60.04 | 8 |
| | ATOM | 4658 | N ILE C 173 | 20.186 | 56.530 | 46.154 | 1.00 | 58.96 | 7 |
| | ATOM | 4659 | CA ILE C 173 | 20.182 | 57.827 | 45.494 | 1.00 | 59.79 | 6 |
| | ATOM | 4660 | CB ILE C 173 | 20.016 | 57.687 | 43.970 | 1.00 | 60.17 | 6 |
| 40 | ATOM | 4661 | CG2 ILE C 173 | 19.918 | 59.071 | 43.334 | 1.00 | 57.73 | 6 |
| | ATOM | 4662 | CG1 ILE C 173 | 21.191 | 56.896 | 43.384 | 1.00 | 59.23 | 6 |
| | ATOM | 4663 | CD1 ILE C 173 | 21.053 | 56.663 | 41.902 | 1.00 | 58.26 | 6 |
| | ATOM | 4664 | C ILE C 173 | 19.088 | 58.756 | 45.977 | 1.00 | 59.99 | 6 |
| | ATOM | 4665 | O ILE C 173 | 17.912 | 58.391 | 46.021 | 1.00 | 57.81 | 8 |
| 45 | ATOM | 4666 | N LEU C 174 | 19.480 | 59.972 | 46.321 | 1.00 | 60.93 | 7 |
| | ATOM | 4667 | CA LEU C 174 | 18.510 | 60.943 | 46.782 | 1.00 | 62.65 | 6 |
| | ATOM | 4668 | CB LEU C 174 | 19.164 | 61.916 | 47.756 | 1.00 | 62.58 | 6 |
| | ATOM | 4669 | CG LEU C 174 | 19.967 | 61.213 | 48.856 | 1.00 | 63.64 | 6 |
| | ATOM | 4670 | CD1 LEU C 174 | 20.647 | 62.264 | 49.723 | 1.00 | 63.25 | 6 |
| 50 | ATOM | 4671 | CD2 LEU C 174 | 19.054 | 60.303 | 49.684 | 1.00 | 61.62 | 6 |
| | ATOM | 4672 | C LEU C 174 | 17.985 | 61.680 | 45.564 | 1.00 | 64.25 | 6 |
| | ATOM | 4673 | O LEU C 174 | 16.781 | 61.734 | 45.329 | 1.00 | 65.71 | 8 |
| | ATOM | 4674 | N ASP C 175 | 18.893 | 62.223 | 44.768 | 1.00 | 65.23 | 7 |
| | ATOM | 4675 | CA ASP C 175 | 18.485 | 62.951 | 43.576 | 1.00 | 66.02 | 6 |
| 55 | ATOM | 4676 | CB ASP C 175 | 17.949 | 64.334 | 43.991 | 1.00 | 67.24 | 6 |
| | ATOM | 4677 | CG ASP C 175 | 17.419 | 65.160 | 42.812 | 1.00 | 68.54 | 6 |
| | ATOM | 4678 | OD1 ASP C 175 | 16.598 | 64.650 | 42.011 | 1.00 | 69.53 | 8 |
| | ATOM | 4679 | OD2 ASP C 175 | 17.812 | 66.338 | 42.695 | 1.00 | 66.59 | 8 |
| | ATOM | 4680 | C ASP C 175 | 19.651 | 63.084 | 42.593 | 1.00 | 66.29 | 6 |
| 60 | ATOM | 4681 | O ASP C 175 | 20.829 | 63.031 | 42.980 | 1.00 | 66.20 | 8 |
| | ATOM | 4682 | N VAL C 176 | 19.312 | 63.237 | 41.318 | 1.00 | 66.07 | 7 |
| | ATOM | 4683 | CA VAL C 176 | 20.308 | 63.391 | 40.267 | 1.00 | 65.83 | 6 |
| | ATOM | 4684 | CB VAL C 176 | 20.426 | 62.109 | 39.401 | 1.00 | 66.59 | 6 |
| | ATOM | 4685 | CG1 VAL C 176 | 21.382 | 62.345 | 38.232 | 1.00 | 64.35 | 6 |
| | ATOM | 4686 | CG2 VAL C 176 | 20.900 | 60.943 | 40.254 | 1.00 | 63.70 | 6 |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 4687 | C VAL C 176 | 19.869 | 64.532 | 39.368 | 1.00 | 67.12 | 6 |
| | ATOM | 4688 | O VAL C 176 | 18.715 | 64.589 | 38.956 | 1.00 | 67.64 | 8 |
| | ATOM | 4689 | N THR C 177 | 20.786 | 65.447 | 39.075 | 1.00 | 68.63 | 7 |
| | ATOM | 4690 | CA THR C 177 | 20.482 | 66.573 | 38.200 | 1.00 | 69.48 | 6 |
| | ATOM | 4691 | CB THR C 177 | 20.215 | 67.861 | 39.004 | 1.00 | 69.26 | 6 |
| 10 | ATOM | 4692 | OG1 THR C 177 | 21.310 | 68.109 | 39.894 | 1.00 | 68.92 | 8 |
| | ATOM | 4693 | CG2 THR C 177 | 18.932 | 67.718 | 39.804 | 1.00 | 68.40 | 6 |
| | ATOM | 4694 | C THR C 177 | 21.640 | 66.813 | 37.245 | 1.00 | 70.44 | 6 |
| | ATOM | 4695 | O THR C 177 | 22.802 | 66.641 | 37.614 | 1.00 | 69.76 | 8 |
| | ATOM | 4696 | N GLN C 178 | 21.312 | 67.207 | 36.018 | 1.00 | 71.94 | 7 |
| 15 | ATOM | 4697 | CA GLN C 178 | 22.320 | 67.470 | 34.998 | 1.00 | 73.43 | 6 |
| | ATOM | 4698 | CB GLN C 178 | 22.150 | 66.500 | 33.831 | 1.00 | 76.20 | 6 |
| | ATOM | 4699 | CG GLN C 178 | 21.560 | 65.148 | 34.220 | 1.00 | 80.00 | 6 |
| | ATOM | 4700 | CD GLN C 178 | 21.896 | 64.046 | 33.196 | 1.00 | 83.21 | 6 |
| | ATOM | 4701 | OE1 GLN C 178 | 21.745 | 64.237 | 31.973 | 1.00 | 84.40 | 8 |
| 20 | ATOM | 4702 | NE2 GLN C 178 | 22.346 | 62.889 | 33.694 | 1.00 | 82.90 | 7 |
| | ATOM | 4703 | C GLN C 178 | 22.149 | 68.884 | 34.482 | 1.00 | 72.16 | 6 |
| | ATOM | 4704 | O GLN C 178 | 21.070 | 69.244 | 34.044 | 1.00 | 72.49 | 8 |
| | ATOM | 4705 | N LYS C 179 | 23.214 | 69.675 | 34.522 | 1.00 | 71.74 | 7 |
| | ATOM | 4706 | CA LYS C 179 | 23.166 | 71.054 | 34.048 | 1.00 | 71.38 | 6 |
| 25 | ATOM | 4707 | CB LYS C 179 | 23.205 | 72.022 | 35.233 | 1.00 | 73.17 | 6 |
| | ATOM | 4708 | CG LYS C 179 | 22.291 | 71.610 | 36.380 | 1.00 | 78.41 | 6 |
| | ATOM | 4709 | CD LYS C 179 | 22.499 | 72.459 | 37.644 | 1.00 | 79.07 | 6 |
| | ATOM | 4710 | CE LYS C 179 | 21.814 | 71.821 | 38.864 | 1.00 | 80.35 | 6 |
| | ATOM | 4711 | NZ LYS C 179 | 22.363 | 70.452 | 39.163 | 1.00 | 81.10 | 7 |
| 30 | ATOM | 4712 | C LYS C 179 | 24.384 | 71.301 | 33.176 | 1.00 | 70.13 | 6 |
| | ATOM | 4713 | O LYS C 179 | 25.504 | 71.353 | 33.681 | 1.00 | 70.65 | 8 |
| | ATOM | 4714 | N LYS C 180 | 24.180 | 71.466 | 31.876 | 1.00 | 68.21 | 7 |
| | ATOM | 4715 | CA LYS C 180 | 25.306 | 71.719 | 30.978 | 1.00 | 67.25 | 6 |
| | ATOM | 4716 | CB LYS C 180 | 24.833 | 71.667 | 29.519 | 1.00 | 67.12 | 6 |
| 35 | ATOM | 4717 | CG LYS C 180 | 24.008 | 72.846 | 29.053 | 1.00 | 63.90 | 6 |
| | ATOM | 4718 | CD LYS C 180 | 24.908 | 73.920 | 28.488 | 1.00 | 63.70 | 6 |
| | ATOM | 4719 | CE LYS C 180 | 25.645 | 73.452 | 27.223 | 1.00 | 63.89 | 6 |
| | ATOM | 4720 | NZ LYS C 180 | 24.768 | 73.295 | 26.013 | 1.00 | 62.80 | 7 |
| | ATOM | 4721 | C LYS C 180 | 25.971 | 73.075 | 31.266 | 1.00 | 67.33 | 6 |
| 40 | ATOM | 4722 | O LYS C 180 | 25.552 | 73.803 | 32.160 | 1.00 | 66.68 | 8 |
| | ATOM | 4723 | N ASN C 181 | 27.027 | 73.399 | 30.528 | 1.00 | 67.89 | 7 |
| | ATOM | 4724 | CA ASN C 181 | 27.698 | 74.674 | 30.702 | 1.00 | 67.78 | 6 |
| | ATOM | 4725 | CB ASN C 181 | 27.967 | 74.948 | 32.191 | 1.00 | 69.90 | 6 |
| | ATOM | 4726 | CG ASN C 181 | 28.580 | 73.770 | 32.916 | 1.00 | 70.82 | 6 |
| 45 | ATOM | 4727 | OD1 ASN C 181 | 29.508 | 73.137 | 32.422 | 1.00 | 73.77 | 8 |
| | ATOM | 4728 | ND2 ASN C 181 | 28.071 | 73.481 | 34.109 | 1.00 | 70.00 | 7 |
| | ATOM | 4729 | C ASN C 181 | 28.977 | 74.884 | 29.901 | 1.00 | 67.29 | 6 |
| | ATOM | 4730 | O ASN C 181 | 29.937 | 74.153 | 30.049 | 1.00 | 68.57 | 8 |
| | ATOM | 4731 | N SER C 182 | 28.978 | 75.911 | 29.058 | 1.00 | 67.43 | 7 |
| 50 | ATOM | 4732 | CA SER C 182 | 30.134 | 76.248 | 28.233 | 1.00 | 66.28 | 6 |
| | ATOM | 4733 | CB SER C 182 | 29.726 | 77.290 | 27.186 | 1.00 | 65.32 | 6 |
| | ATOM | 4734 | OG SER C 182 | 30.731 | 77.477 | 26.214 | 1.00 | 68.09 | 8 |
| | ATOM | 4735 | C SER C 182 | 31.230 | 76.798 | 29.141 | 1.00 | 65.83 | 6 |
| | ATOM | 4736 | O SER C 182 | 30.941 | 77.272 | 30.231 | 1.00 | 66.92 | 8 |
| 55 | ATOM | 4737 | N VAL C 183 | 32.483 | 76.731 | 28.698 | 1.00 | 65.76 | 7 |
| | ATOM | 4738 | CA VAL C 183 | 33.613 | 77.211 | 29.498 | 1.00 | 65.65 | 6 |
| | ATOM | 4739 | CB VAL C 183 | 33.872 | 76.264 | 30.696 | 1.00 | 63.98 | 6 |
| | ATOM | 4740 | CG1 VAL C 183 | 33.648 | 74.843 | 30.277 | 1.00 | 64.03 | 6 |
| | ATOM | 4741 | CG2 VAL C 183 | 35.292 | 76.442 | 31.209 | 1.00 | 61.75 | 6 |
| 60 | ATOM | 4742 | C VAL C 183 | 34.925 | 77.375 | 28.728 | 1.00 | 65.88 | 6 |
| | ATOM | 4743 | O VAL C 183 | 35.305 | 76.515 | 27.944 | 1.00 | 65.40 | 8 |
| | ATOM | 4744 | N THR C 184 | 35.616 | 78.485 | 28.957 | 1.00 | 66.99 | 7 |
| | ATOM | 4745 | CA THR C 184 | 36.892 | 78.722 | 28.293 | 1.00 | 68.57 | 6 |
| | ATOM | 4746 | CB THR C 184 | 36.995 | 80.168 | 27.732 | 1.00 | 67.80 | 6 |
| | ATOM | 4747 | OG1 THR C 184 | 35.981 | 80.369 | 26.737 | 1.00 | 66.40 | 8 |

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|----|------|------|---------------|--------|--------|--------|------|-------|----|--|
| 5 | ATOM | 4748 | CG2 THR C 184 | 38.370 | 80.406 | 27.094 | 1.00 | 66.48 | 6 | |
| | ATOM | 4749 | C THR C 184 | 38.032 | 78.470 | 29.292 | 1.00 | 70.57 | 6 | |
| | ATOM | 4750 | O THR C 184 | 37.920 | 78.802 | 30.482 | 1.00 | 70.99 | 8 | |
| | ATOM | 4751 | N TYR C 185 | 39.118 | 77.869 | 28.815 | 1.00 | 70.74 | 7 | |
| | ATOM | 4752 | CA TYR C 185 | 40.236 | 77.572 | 29.683 | 1.00 | 71.98 | 6 | |
| 10 | ATOM | 4753 | CB TYR C 185 | 40.555 | 76.067 | 29.658 | 1.00 | 72.58 | 6 | |
| | ATOM | 4754 | CG TYR C 185 | 39.351 | 75.195 | 29.937 | 1.00 | 72.59 | 6 | |
| | ATOM | 4755 | CD1 TYR C 185 | 38.363 | 75.011 | 28.970 | 1.00 | 73.55 | 6 | |
| | ATOM | 4756 | CE1 TYR C 185 | 37.224 | 74.258 | 29.236 | 1.00 | 72.54 | 6 | |
| | ATOM | 4757 | CD2 TYR C 185 | 39.164 | 74.597 | 31.185 | 1.00 | 72.27 | 6 | |
| 15 | ATOM | 4758 | CE2 TYR C 185 | 38.017 | 73.839 | 31.461 | 1.00 | 71.72 | 6 | |
| | ATOM | 4759 | CZ TYR C 185 | 37.057 | 73.678 | 30.480 | 1.00 | 71.73 | 6 | |
| | ATOM | 4760 | OH TYR C 185 | 35.920 | 72.951 | 30.732 | 1.00 | 71.36 | 8 | |
| | ATOM | 4761 | C TYR C 185 | 41.426 | 78.355 | 29.191 | 1.00 | 73.72 | 6 | |
| | ATOM | 4762 | O TYR C 185 | 41.625 | 78.492 | 27.983 | 1.00 | 74.41 | 8 | |
| 20 | ATOM | 4763 | N SER C 186 | 42.220 | 78.869 | 30.125 | 1.00 | 75.63 | 7 | |
| | ATOM | 4764 | CA SER C 186 | 43.405 | 79.653 | 29.772 | 1.00 | 77.64 | 6 | |
| | ATOM | 4765 | CB SER C 186 | 44.183 | 80.015 | 31.043 | 1.00 | 77.47 | 6 | |
| | ATOM | 4766 | OG SER C 186 | 44.398 | 78.870 | 31.858 | 1.00 | 78.93 | 8 | |
| | ATOM | 4767 | C SER C 186 | 44.300 | 78.875 | 28.793 | 1.00 | 77.75 | 6 | |
| 25 | ATOM | 4768 | O SER C 186 | 44.926 | 79.457 | 27.893 | 1.00 | 76.44 | 8 | |
| | ATOM | 4769 | N CYS C 187 | 44.332 | 77.556 | 28.977 | 1.00 | 78.65 | 7 | |
| | ATOM | 4770 | CA CYS C 187 | 45.116 | 76.648 | 28.135 | 1.00 | 79.38 | 6 | |
| | ATOM | 4771 | C CYS C 187 | 44.658 | 76.703 | 26.715 | 1.00 | 79.55 | 6 | |
| | ATOM | 4772 | O CYS C 187 | 45.443 | 76.687 | 25.771 | 1.00 | 79.09 | 8 | |
| 30 | ATOM | 4773 | CB CYS C 187 | 44.899 | 75.178 | 28.529 | 1.00 | 79.04 | 6 | |
| | ATOM | 4774 | SG CYS C 187 | 43.205 | 74.462 | 28.241 | 1.00 | 80.14 | 16 | |
| | ATOM | 4775 | N CYS C 188 | 43.345 | 76.774 | 26.589 | 1.00 | 80.45 | 7 | |
| | ATOM | 4776 | CA CYS C 188 | 42.727 | 76.642 | 25.305 | 1.00 | 79.63 | 6 | |
| | ATOM | 4777 | C CYS C 188 | 41.779 | 77.755 | 24.835 | 1.00 | 79.24 | 6 | |
| 35 | ATOM | 4778 | O CYS C 188 | 40.785 | 78.065 | 25.504 | 1.00 | 81.46 | 8 | |
| | ATOM | 4779 | CB CYS C 188 | 42.037 | 75.269 | 25.365 | 1.00 | 79.66 | 6 | |
| | ATOM | 4780 | SG CYS C 188 | 42.984 | 73.940 | 26.264 | 1.00 | 75.61 | 16 | |
| | ATOM | 4781 | N PRO C 189 | 42.070 | 78.346 | 23.656 | 1.00 | 77.55 | 7 | |
| | ATOM | 4782 | CD PRO C 189 | 43.222 | 77.849 | 22.879 | 1.00 | 76.91 | 6 | |
| 40 | ATOM | 4783 | CA PRO C 189 | 41.378 | 79.431 | 22.922 | 1.00 | 75.67 | 6 | |
| | ATOM | 4784 | CB PRO C 189 | 41.921 | 79.283 | 21.502 | 1.00 | 75.82 | 6 | |
| | ATOM | 4785 | CG PRO C 189 | 43.328 | 78.858 | 21.747 | 1.00 | 77.27 | 6 | |
| | ATOM | 4786 | C PRO C 189 | 39.835 | 79.468 | 22.927 | 1.00 | 73.97 | 6 | |
| | ATOM | 4787 | O PRO C 189 | 39.233 | 80.403 | 23.459 | 1.00 | 73.90 | 8 | |
| 45 | ATOM | 4788 | N GLU C 190 | 39.201 | 78.465 | 22.317 | 1.00 | 71.85 | 7 | |
| | ATOM | 4789 | CA GLU C 190 | 37.734 | 78.404 | 22.246 | 1.00 | 68.61 | 6 | |
| | ATOM | 4790 | CB GLU C 190 | 37.305 | 77.497 | 21.099 | 1.00 | 70.45 | 6 | |
| | ATOM | 4791 | CG GLU C 190 | 38.277 | 77.434 | 19.945 | 1.00 | 72.05 | 6 | |
| | ATOM | 4792 | CD GLU C 190 | 38.082 | 78.554 | 18.969 | 1.00 | 73.59 | 6 | |
| 50 | ATOM | 4793 | OE1 GLU C 190 | 36.908 | 78.876 | 18.657 | 1.00 | 73.46 | 8 | |
| | ATOM | 4794 | OE2 GLU C 190 | 39.106 | 79.100 | 18.504 | 1.00 | 77.52 | 8 | |
| | ATOM | 4795 | C GLU C 190 | 37.084 | 77.889 | 23.528 | 1.00 | 64.48 | 6 | |
| | ATOM | 4796 | O GLU C 190 | 37.762 | 77.596 | 24.501 | 1.00 | 64.47 | 8 | |
| | ATOM | 4797 | N ALA C 191 | 35.764 | 77.765 | 23.514 | 1.00 | 60.72 | 7 | |
| 55 | ATOM | 4798 | CA ALA C 191 | 35.035 | 77.281 | 24.679 | 1.00 | 60.54 | 6 | |
| | ATOM | 4799 | CB ALA C 191 | 33.755 | 78.075 | 24.854 | 1.00 | 59.52 | 6 | |
| | ATOM | 4800 | C ALA C 191 | 34.702 | 75.796 | 24.554 | 1.00 | 60.66 | 6 | |
| | ATOM | 4801 | O ALA C 191 | 34.423 | 75.306 | 23.458 | 1.00 | 60.77 | 8 | |
| | ATOM | 4802 | N TYR C 192 | 34.717 | 75.080 | 25.675 | 1.00 | 58.74 | 7 | |
| 60 | ATOM | 4803 | CA TYR C 192 | 34.409 | 73.653 | 25.659 | 1.00 | 57.24 | 6 | |
| | ATOM | 4804 | CB TYR C 192 | 35.621 | 72.826 | 26.109 | 1.00 | 55.18 | 6 | |
| | ATOM | 4805 | CG TYR C 192 | 36.737 | 72.825 | 25.097 | 1.00 | 55.96 | 6 | |
| | ATOM | 4806 | CD1 TYR C 192 | 37.694 | 73.842 | 25.075 | 1.00 | 56.31 | 6 | |
| | ATOM | 4807 | CE1 TYR C 192 | 38.680 | 73.887 | 24.092 | 1.00 | 56.74 | 6 | |
| | ATOM | 4808 | CD2 TYR C 192 | 36.800 | 71.844 | 24.109 | 1.00 | 56.77 | 6 | |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 4809 | CE2 TYR C 192 | 37.785 | 71.874 | 23.121 | 1.00 | 57.49 | 6 | |
| | ATOM | 4810 | CZ TYR C 192 | 38.720 | 72.898 | 23.119 | 1.00 | 58.13 | 6 | |
| | ATOM | 4811 | OH TYR C 192 | 39.689 | 72.918 | 22.148 | 1.00 | 58.55 | 8 | |
| | ATOM | 4812 | C TYR C 192 | 33.204 | 73.295 | 26.508 | 1.00 | 57.26 | 6 | |
| | ATOM | 4813 | O TYR C 192 | 33.292 | 73.241 | 27.736 | 1.00 | 57.40 | 8 | |
| 10 | ATOM | 4814 | N GLU C 193 | 32.084 | 73.042 | 25.836 | 1.00 | 57.28 | 7 | |
| | ATOM | 4815 | CA GLU C 193 | 30.839 | 72.678 | 26.506 | 1.00 | 58.77 | 6 | |
| | ATOM | 4816 | CB GLU C 193 | 29.681 | 72.597 | 25.495 | 1.00 | 59.02 | 6 | |
| | ATOM | 4817 | CG GLU C 193 | 29.342 | 73.912 | 24.823 | 1.00 | 61.64 | 6 | |
| | ATOM | 4818 | CD GLU C 193 | 28.118 | 73.827 | 23.945 | 1.00 | 63.79 | 6 | |
| 15 | ATOM | 4819 | OE1 GLU C 193 | 27.107 | 73.242 | 24.411 | 1.00 | 66.05 | 8 | |
| | ATOM | 4820 | OE2 GLU C 193 | 28.171 | 74.355 | 22.805 | 1.00 | 63.82 | 8 | |
| | ATOM | 4821 | C GLU C 193 | 30.968 | 71.336 | 27.224 | 1.00 | 58.56 | 6 | |
| | ATOM | 4822 | O GLU C 193 | 31.749 | 70.471 | 26.811 | 1.00 | 58.35 | 8 | |
| | ATOM | 4823 | N ASP C 194 | 30.197 | 71.171 | 28.296 | 1.00 | 57.04 | 7 | |
| 20 | ATOM | 4824 | CA ASP C 194 | 30.215 | 69.940 | 29.059 | 1.00 | 57.30 | 6 | |
| | ATOM | 4825 | CB ASP C 194 | 31.473 | 69.849 | 29.932 | 1.00 | 58.11 | 6 | |
| | ATOM | 4826 | CG ASP C 194 | 31.430 | 70.777 | 31.141 | 1.00 | 58.91 | 6 | |
| | ATOM | 4827 | OD1 ASP C 194 | 32.220 | 71.742 | 31.172 | 1.00 | 57.40 | 8 | |
| | ATOM | 4828 | OD2 ASP C 194 | 30.614 | 70.538 | 32.060 | 1.00 | 58.46 | 8 | |
| 25 | ATOM | 4829 | C ASP C 194 | 28.982 | 69.848 | 29.933 | 1.00 | 56.78 | 6 | |
| | ATOM | 4830 | O ASP C 194 | 28.411 | 70.864 | 30.320 | 1.00 | 56.90 | 8 | |
| | ATOM | 4831 | N VAL C 195 | 28.567 | 68.619 | 30.223 | 1.00 | 55.47 | 7 | |
| | ATOM | 4832 | CA VAL C 195 | 27.404 | 68.373 | 31.061 | 1.00 | 55.52 | 6 | |
| | ATOM | 4833 | CB VAL C 195 | 26.538 | 67.236 | 30.504 | 1.00 | 54.50 | 6 | |
| 30 | ATOM | 4834 | CG1 VAL C 195 | 25.469 | 66.841 | 31.511 | 1.00 | 52.44 | 6 | |
| | ATOM | 4835 | CG2 VAL C 195 | 25.914 | 67.671 | 29.199 | 1.00 | 55.96 | 6 | |
| | ATOM | 4836 | C VAL C 195 | 27.874 | 67.973 | 32.444 | 1.00 | 56.12 | 6 | |
| | ATOM | 4837 | O VAL C 195 | 28.661 | 67.046 | 32.602 | 1.00 | 56.74 | 8 | |
| | ATOM | 4838 | N GLU C 196 | 27.388 | 68.675 | 33.451 | 1.00 | 56.91 | 7 | |
| 35 | ATOM | 4839 | CA GLU C 196 | 27.777 | 68.370 | 34.816 | 1.00 | 57.46 | 6 | |
| | ATOM | 4840 | CB GLU C 196 | 28.051 | 69.654 | 35.581 | 1.00 | 58.09 | 6 | |
| | ATOM | 4841 | CG GLU C 196 | 28.548 | 69.445 | 36.972 | 1.00 | 59.59 | 6 | |
| | ATOM | 4842 | CD GLU C 196 | 28.730 | 70.758 | 37.700 | 1.00 | 62.33 | 6 | |
| | ATOM | 4843 | OE1 GLU C 196 | 29.523 | 71.594 | 37.229 | 1.00 | 62.53 | 8 | |
| 40 | ATOM | 4844 | OE2 GLU C 196 | 28.074 | 70.958 | 38.746 | 1.00 | 65.85 | 8 | |
| | ATOM | 4845 | C GLU C 196 | 26.636 | 67.627 | 35.453 | 1.00 | 57.05 | 6 | |
| | ATOM | 4846 | O GLU C 196 | 25.517 | 68.120 | 35.487 | 1.00 | 59.06 | 8 | |
| | ATOM | 4847 | N VAL C 197 | 26.914 | 66.427 | 35.938 | 1.00 | 56.46 | 7 | |
| | ATOM | 4848 | CA VAL C 197 | 25.889 | 65.612 | 36.566 | 1.00 | 55.58 | 6 | |
| 45 | ATOM | 4849 | CB VAL C 197 | 25.867 | 64.179 | 35.984 | 1.00 | 53.38 | 6 | |
| | ATOM | 4850 | CG1 VAL C 197 | 24.777 | 63.360 | 36.649 | 1.00 | 50.20 | 6 | |
| | ATOM | 4851 | CG2 VAL C 197 | 25.629 | 64.239 | 34.486 | 1.00 | 51.56 | 6 | |
| | ATOM | 4852 | C VAL C 197 | 26.199 | 65.546 | 38.041 | 1.00 | 56.50 | 6 | |
| | ATOM | 4853 | O VAL C 197 | 27.320 | 65.207 | 38.430 | 1.00 | 58.31 | 8 | |
| 50 | ATOM | 4854 | N SER C 198 | 25.214 | 65.885 | 38.866 | 1.00 | 57.35 | 7 | |
| | ATOM | 4855 | CA SER C 198 | 25.407 | 65.857 | 40.309 | 1.00 | 57.08 | 6 | |
| | ATOM | 4856 | CB SER C 198 | 24.867 | 67.137 | 40.943 | 1.00 | 56.30 | 6 | |
| | ATOM | 4857 | OG SER C 198 | 25.661 | 68.246 | 40.565 | 1.00 | 55.97 | 8 | |
| | ATOM | 4858 | C SER C 198 | 24.717 | 64.643 | 40.886 | 1.00 | 57.36 | 6 | |
| 55 | ATOM | 4859 | O SER C 198 | 23.513 | 64.460 | 40.731 | 1.00 | 58.49 | 8 | |
| | ATOM | 4860 | N LEU C 199 | 25.494 | 63.791 | 41.531 | 1.00 | 57.83 | 7 | |
| | ATOM | 4861 | CA LEU C 199 | 24.938 | 62.594 | 42.120 | 1.00 | 57.20 | 6 | |
| | ATOM | 4862 | CB LEU C 199 | 25.824 | 61.383 | 41.834 | 1.00 | 56.00 | 6 | |
| | ATOM | 4863 | CG LEU C 199 | 25.457 | 60.110 | 42.606 | 1.00 | 56.43 | 6 | |
| 60 | ATOM | 4864 | CD1 LEU C 199 | 24.073 | 59.627 | 42.211 | 1.00 | 53.65 | 6 | |
| | ATOM | 4865 | CD2 LEU C 199 | 26.487 | 59.050 | 42.325 | 1.00 | 55.64 | 6 | |
| | ATOM | 4866 | C LEU C 199 | 24.818 | 62.782 | 43.613 | 1.00 | 58.48 | 6 | |
| | ATOM | 4867 | O LEU C 199 | 25.819 | 62.737 | 44.337 | 1.00 | 59.73 | 8 | |
| | ATOM | 4868 | N ASN C 200 | 23.593 | 63.012 | 44.070 | 1.00 | 58.64 | 7 | |
| | ATOM | 4869 | CA ASN C 200 | 23.355 | 63.168 | 45.489 | 1.00 | 58.44 | 6 | |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 4870 | CB ASN C 200 | 22.285 | 64.232 | 45.754 | 1.00 | 60.17 | 6 | |
| | ATOM | 4871 | CG ASN C 200 | 21.985 | 64.387 | 47.239 | 1.00 | 62.50 | 6 | |
| | ATOM | 4872 | OD1 ASN C 200 | 22.905 | 64.419 | 48.070 | 1.00 | 64.15 | 8 | |
| | ATOM | 4873 | ND2 ASN C 200 | 20.700 | 64.480 | 47.583 | 1.00 | 61.21 | 7 | |
| | ATOM | 4874 | C ASN C 200 | 22.898 | 61.801 | 45.988 | 1.00 | 55.97 | 6 | |
| 10 | ATOM | 4875 | O ASN C 200 | 21.821 | 61.316 | 45.627 | 1.00 | 54.75 | 8 | |
| | ATOM | 4876 | N PHE C 201 | 23.739 | 61.181 | 46.802 | 1.00 | 53.51 | 7 | |
| | ATOM | 4877 | CA PHE C 201 | 23.454 | 59.867 | 47.330 | 1.00 | 53.54 | 6 | |
| | ATOM | 4878 | CB PHE C 201 | 24.169 | 58.807 | 46.503 | 1.00 | 50.74 | 6 | |
| | ATOM | 4879 | CG PHE C 201 | 25.663 | 58.820 | 46.677 | 1.00 | 48.36 | 6 | |
| 15 | ATOM | 4880 | CD1 PHE C 201 | 26.312 | 57.763 | 47.309 | 1.00 | 45.72 | 6 | |
| | ATOM | 4881 | CD2 PHE C 201 | 26.413 | 59.912 | 46.252 | 1.00 | 46.85 | 6 | |
| | ATOM | 4882 | CE1 PHE C 201 | 27.689 | 57.794 | 47.521 | 1.00 | 43.95 | 6 | |
| | ATOM | 4883 | CE2 PHE C 201 | 27.782 | 59.955 | 46.457 | 1.00 | 45.93 | 6 | |
| | ATOM | 4884 | CZ PHE C 201 | 28.425 | 58.889 | 47.096 | 1.00 | 44.09 | 6 | |
| 20 | ATOM | 4885 | C PHE C 201 | 23.979 | 59.812 | 48.749 | 1.00 | 55.36 | 6 | |
| | ATOM | 4886 | O PHE C 201 | 24.640 | 60.739 | 49.210 | 1.00 | 53.66 | 8 | |
| | ATOM | 4887 | N ARG C 202 | 23.698 | 58.702 | 49.425 | 1.00 | 57.35 | 7 | |
| | ATOM | 4888 | CA ARG C 202 | 24.140 | 58.511 | 50.792 | 1.00 | 59.95 | 6 | |
| | ATOM | 4889 | CB ARG C 202 | 23.192 | 59.224 | 51.744 | 1.00 | 62.36 | 6 | |
| 25 | ATOM | 4890 | CG ARG C 202 | 21.844 | 58.529 | 51.789 | 1.00 | 64.26 | 6 | |
| | ATOM | 4891 | CD ARG C 202 | 20.831 | 59.278 | 52.610 | 1.00 | 67.26 | 6 | |
| | ATOM | 4892 | NE ARG C 202 | 19.555 | 58.567 | 52.620 | 1.00 | 70.54 | 7 | |
| | ATOM | 4893 | CZ ARG C 202 | 18.430 | 59.062 | 53.129 | 1.00 | 69.46 | 6 | |
| | ATOM | 4894 | NH1 ARG C 202 | 18.420 | 60.270 | 53.670 | 1.00 | 69.25 | 7 | |
| 30 | ATOM | 4895 | NH2 ARG C 202 | 17.315 | 58.349 | 53.095 | 1.00 | 69.56 | 7 | |
| | ATOM | 4896 | C ARG C 202 | 24.116 | 57.023 | 51.119 | 1.00 | 60.80 | 6 | |
| | ATOM | 4897 | O ARG C 202 | 23.439 | 56.231 | 50.445 | 1.00 | 60.45 | 8 | |
| | ATOM | 4898 | N LYS C 203 | 24.860 | 56.651 | 52.158 | 1.00 | 61.42 | 7 | |
| | ATOM | 4899 | CA LYS C 203 | 24.886 | 55.270 | 52.603 | 1.00 | 60.82 | 6 | |
| 35 | ATOM | 4900 | CB LYS C 203 | 25.931 | 55.088 | 53.703 | 1.00 | 59.66 | 6 | |
| | ATOM | 4901 | CG LYS C 203 | 25.988 | 53.688 | 54.258 | 1.00 | 61.19 | 6 | |
| | ATOM | 4902 | CD LYS C 203 | 26.955 | 53.617 | 55.404 | 1.00 | 63.27 | 6 | |
| | ATOM | 4903 | CE LYS C 203 | 27.036 | 52.209 | 55.947 | 1.00 | 66.98 | 6 | |
| | ATOM | 4904 | NZ LYS C 203 | 27.621 | 51.250 | 54.945 | 1.00 | 68.80 | 7 | |
| 40 | ATOM | 4905 | C LYS C 203 | 23.477 | 55.037 | 53.157 | 1.00 | 60.81 | 6 | |
| | ATOM | 4906 | O LYS C 203 | 22.878 | 55.942 | 53.735 | 1.00 | 60.52 | 8 | |
| | ATOM | 4907 | N LYS C 204 | 22.913 | 53.858 | 52.944 | 1.00 | 60.36 | 7 | |
| | ATOM | 4908 | CA LYS C 204 | 21.584 | 53.606 | 53.466 | 1.00 | 60.22 | 6 | |
| | ATOM | 4909 | CB LYS C 204 | 21.017 | 52.329 | 52.837 | 1.00 | 58.64 | 6 | |
| 45 | ATOM | 4910 | CG LYS C 204 | 20.591 | 52.487 | 51.381 | 1.00 | 55.82 | 6 | |
| | ATOM | 4911 | CD LYS C 204 | 20.445 | 51.140 | 50.692 | 1.00 | 51.95 | 6 | |
| | ATOM | 4912 | CE LYS C 204 | 19.975 | 51.298 | 49.253 | 1.00 | 52.70 | 6 | |
| | ATOM | 4913 | NZ LYS C 204 | 19.967 | 50.027 | 48.458 | 1.00 | 51.76 | 7 | |
| | ATOM | 4914 | C LYS C 204 | 21.742 | 53.460 | 54.977 | 1.00 | 62.01 | 6 | |
| 50 | ATOM | 4915 | O LYS C 204 | 22.711 | 52.854 | 55.440 | 1.00 | 63.36 | 8 | |
| | ATOM | 4916 | N GLY C 205 | 20.811 | 54.022 | 55.747 | 1.00 | 62.55 | 7 | |
| | ATOM | 4917 | CA GLY C 205 | 20.898 | 53.921 | 57.202 | 1.00 | 62.30 | 6 | |
| | ATOM | 4918 | C GLY C 205 | 19.797 | 53.078 | 57.844 | 1.00 | 61.75 | 6 | |
| | ATOM | 4919 | OT1 GLY C 205 | 18.911 | 52.614 | 57.093 | 1.00 | 60.18 | 8 | |
| 55 | ATOM | 4920 | OT2 GLY C 205 | 19.811 | 52.879 | 59.092 | 1.00 | 60.86 | 8 | |
| | ATOM | 4921 | CB PHE D 1 | 39.182 | 71.754 | 1.648 | 1.00 | 71.47 | 6 | |
| | ATOM | 4922 | CG PHE D 1 | 40.239 | 71.385 | 0.623 | 1.00 | 73.60 | 6 | |
| | ATOM | 4923 | CD1 PHE D 1 | 40.122 | 70.241 | -0.169 | 1.00 | 75.22 | 6 | |
| | ATOM | 4924 | CD2 PHE D 1 | 41.397 | 72.176 | 0.493 | 1.00 | 73.83 | 6 | |
| 60 | ATOM | 4925 | CE1 PHE D 1 | 41.141 | 69.886 | -1.081 | 1.00 | 75.00 | 6 | |
| | ATOM | 4926 | CE2 PHE D 1 | 42.418 | 71.835 | -0.410 | 1.00 | 73.07 | 6 | |
| | ATOM | 4927 | CZ PHE D 1 | 42.289 | 70.688 | -1.199 | 1.00 | 74.63 | 6 | |
| | ATOM | 4928 | C PHE D 1 | 37.071 | 70.999 | 2.658 | 1.00 | 68.35 | 6 | |
| | ATOM | 4929 | O PHE D 1 | 37.607 | 71.392 | 3.688 | 1.00 | 69.33 | 8 | |
| | ATOM | 4930 | N PHE D 1 | 37.010 | 72.284 | 0.515 | 1.00 | 69.08 | 7 | |

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|----|------|------|-----|-----|---|---|--------|--------|--------|------|-------|---|
| | ATOM | 4931 | CA | PHE | D | 1 | 37.756 | 71.268 | 1.321 | 1.00 | 69.54 | 6 |
| | ATOM | 4932 | N | ASP | D | 2 | 35.915 | 70.338 | 2.678 | 1.00 | 67.84 | 7 |
| | ATOM | 4933 | CA | ASP | D | 2 | 35.253 | 70.061 | 3.967 | 1.00 | 66.03 | 6 |
| | ATOM | 4934 | CB | ASP | D | 2 | 33.949 | 69.266 | 3.772 | 1.00 | 66.47 | 6 |
| 5 | ATOM | 4935 | CG | ASP | D | 2 | 34.138 | 68.032 | 2.928 | 1.00 | 68.89 | 6 |
| | ATOM | 4936 | OD1 | ASP | D | 2 | 35.029 | 67.218 | 3.287 | 1.00 | 68.16 | 8 |
| | ATOM | 4937 | OD2 | ASP | D | 2 | 33.396 | 67.886 | 1.912 | 1.00 | 70.47 | 8 |
| | ATOM | 4938 | C | ASP | D | 2 | 36.181 | 69.310 | 4.933 | 1.00 | 64.63 | 6 |
| | ATOM | 4939 | O | ASP | D | 2 | 37.378 | 69.165 | 4.672 | 1.00 | 64.43 | 8 |
| 10 | ATOM | 4940 | N | ARG | D | 3 | 35.639 | 68.837 | 6.049 | 1.00 | 62.26 | 7 |
| | ATOM | 4941 | CA | ARG | D | 3 | 36.461 | 68.128 | 7.029 | 1.00 | 60.44 | 6 |
| | ATOM | 4942 | CB | ARG | D | 3 | 35.748 | 68.078 | 8.388 | 1.00 | 60.90 | 6 |
| | ATOM | 4943 | CG | ARG | D | 3 | 36.068 | 69.254 | 9.302 | 1.00 | 60.80 | 6 |
| | ATOM | 4944 | CD | ARG | D | 3 | 35.185 | 69.243 | 10.532 | 1.00 | 65.18 | 6 |
| 15 | ATOM | 4945 | NE | ARG | D | 3 | 35.849 | 69.838 | 11.696 | 1.00 | 66.90 | 7 |
| | ATOM | 4946 | CZ | ARG | D | 3 | 36.028 | 71.141 | 11.888 | 1.00 | 66.63 | 6 |
| | ATOM | 4947 | NH1 | ARG | D | 3 | 35.591 | 72.031 | 11.002 | 1.00 | 68.16 | 7 |
| | ATOM | 4948 | NH2 | ARG | D | 3 | 36.664 | 71.553 | 12.964 | 1.00 | 66.33 | 7 |
| | ATOM | 4949 | C | ARG | D | 3 | 36.831 | 66.719 | 6.580 | 1.00 | 59.10 | 6 |
| 20 | ATOM | 4950 | O | ARG | D | 3 | 37.938 | 66.252 | 6.845 | 1.00 | 57.28 | 8 |
| | ATOM | 4951 | N | ALA | D | 4 | 35.909 | 66.050 | 5.891 | 1.00 | 56.67 | 7 |
| | ATOM | 4952 | CA | ALA | D | 4 | 36.153 | 64.699 | 5.414 | 1.00 | 53.48 | 6 |
| | ATOM | 4953 | CB | ALA | D | 4 | 34.938 | 64.175 | 4.706 | 1.00 | 52.26 | 6 |
| | ATOM | 4954 | C | ALA | D | 4 | 37.347 | 64.696 | 4.479 | 1.00 | 53.39 | 6 |
| 25 | ATOM | 4955 | O | ALA | D | 4 | 38.225 | 63.851 | 4.600 | 1.00 | 52.40 | 8 |
| | ATOM | 4956 | N | ASP | D | 5 | 37.381 | 65.650 | 3.550 | 1.00 | 54.53 | 7 |
| | ATOM | 4957 | CA | ASP | D | 5 | 38.489 | 65.756 | 2.602 | 1.00 | 55.71 | 6 |
| | ATOM | 4958 | CB | ASP | D | 5 | 38.266 | 66.914 | 1.627 | 1.00 | 58.22 | 6 |
| | ATOM | 4959 | CG | ASP | D | 5 | 36.938 | 66.810 | 0.881 | 1.00 | 61.46 | 6 |
| 30 | ATOM | 4960 | OD1 | ASP | D | 5 | 36.605 | 65.709 | 0.386 | 1.00 | 64.32 | 8 |
| | ATOM | 4961 | OD2 | ASP | D | 5 | 36.227 | 67.832 | 0.773 | 1.00 | 63.22 | 8 |
| | ATOM | 4962 | C | ASP | D | 5 | 39.816 | 65.970 | 3.326 | 1.00 | 54.28 | 6 |
| | ATOM | 4963 | O | ASP | D | 5 | 40.844 | 65.440 | 2.914 | 1.00 | 52.86 | 8 |
| | ATOM | 4964 | N | ILE | D | 6 | 39.787 | 66.735 | 4.410 | 1.00 | 52.53 | 7 |
| 35 | ATOM | 4965 | CA | ILE | D | 6 | 41.007 | 67.003 | 5.154 | 1.00 | 53.69 | 6 |
| | ATOM | 4966 | CB | ILE | D | 6 | 40.813 | 68.128 | 6.191 | 1.00 | 55.79 | 6 |
| | ATOM | 4967 | CG2 | ILE | D | 6 | 42.152 | 68.435 | 6.877 | 1.00 | 54.61 | 6 |
| | ATOM | 4968 | CG1 | ILE | D | 6 | 40.266 | 69.385 | 5.499 | 1.00 | 55.83 | 6 |
| | ATOM | 4969 | CD1 | ILE | D | 6 | 40.121 | 70.597 | 6.400 | 1.00 | 55.01 | 6 |
| 40 | ATOM | 4970 | C | ILE | D | 6 | 41.545 | 65.775 | 5.870 | 1.00 | 52.43 | 6 |
| | ATOM | 4971 | O | ILE | D | 6 | 42.711 | 65.420 | 5.709 | 1.00 | 52.78 | 8 |
| | ATOM | 4972 | N | LEU | D | 7 | 40.701 | 65.134 | 6.666 | 1.00 | 51.01 | 7 |
| | ATOM | 4973 | CA | LEU | D | 7 | 41.111 | 63.949 | 7.401 | 1.00 | 50.01 | 6 |
| | ATOM | 4974 | CB | LEU | D | 7 | 39.962 | 63.459 | 8.276 | 1.00 | 47.85 | 6 |
| 45 | ATOM | 4975 | CG | LEU | D | 7 | 39.608 | 64.420 | 9.408 | 1.00 | 46.02 | 6 |
| | ATOM | 4976 | CD1 | LEU | D | 7 | 38.267 | 64.084 | 10.010 | 1.00 | 48.59 | 6 |
| | ATOM | 4977 | CD2 | LEU | D | 7 | 40.687 | 64.356 | 10.440 | 1.00 | 45.91 | 6 |
| | ATOM | 4978 | C | LEU | D | 7 | 41.526 | 62.871 | 6.415 | 1.00 | 51.80 | 6 |
| | ATOM | 4979 | O | LEU | D | 7 | 42.507 | 62.154 | 6.631 | 1.00 | 52.35 | 8 |
| 50 | ATOM | 4980 | N | TYR | D | 8 | 40.788 | 62.781 | 5.315 | 1.00 | 52.55 | 7 |
| | ATOM | 4981 | CA | TYR | D | 8 | 41.060 | 61.788 | 4.288 | 1.00 | 53.16 | 6 |
| | ATOM | 4982 | CB | TYR | D | 8 | 40.047 | 61.936 | 3.159 | 1.00 | 54.45 | 6 |
| | ATOM | 4983 | CG | TYR | D | 8 | 40.294 | 61.006 | 2.006 | 1.00 | 57.19 | 6 |
| | ATOM | 4984 | CD1 | TYR | D | 8 | 40.030 | 59.646 | 2.120 | 1.00 | 57.12 | 6 |
| 55 | ATOM | 4985 | CE1 | TYR | D | 8 | 40.308 | 58.772 | 1.069 | 1.00 | 60.62 | 6 |
| | ATOM | 4986 | CD2 | TYR | D | 8 | 40.841 | 61.481 | 0.810 | 1.00 | 58.57 | 6 |
| | ATOM | 4987 | CE2 | TYR | D | 8 | 41.130 | 60.617 | -0.247 | 1.00 | 60.35 | 6 |
| | ATOM | 4988 | CZ | TYR | D | 8 | 40.863 | 59.264 | -0.112 | 1.00 | 61.47 | 6 |
| | ATOM | 4989 | OH | TYR | D | 8 | 41.162 | 58.403 | -1.149 | 1.00 | 62.53 | 8 |
| 60 | ATOM | 4990 | C | TYR | D | 8 | 42.483 | 61.905 | 3.735 | 1.00 | 53.38 | 6 |
| | ATOM | 4991 | O | TYR | D | 8 | 43.190 | 60.907 | 3.591 | 1.00 | 53.74 | 8 |

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|----|------|------|-----|-----|---|------|--------|--------|--------|--------------|
| 5 | ATOM | 4992 | N | ASN | D | 9 | 42.900 | 63.121 | 3.416 | 1.00 53.53 7 |
| | ATOM | 4993 | CA | ASN | D | 9 | 44.238 | 63.329 | 2.890 | 1.00 55.79 6 |
| | ATOM | 4994 | CB | ASN | D | 9 | 44.451 | 64.800 | 2.509 | 1.00 59.06 6 |
| | ATOM | 4995 | CG | ASN | D | 9 | 43.588 | 65.232 | 1.317 | 1.00 63.96 6 |
| | ATOM | 4996 | OD1 | ASN | D | 9 | 42.912 | 64.406 | 0.688 | 1.00 67.47 8 |
| 10 | ATOM | 4997 | ND2 | ASN | D | 9 | 43.612 | 66.527 | 1.000 | 1.00 65.39 7 |
| | ATOM | 4998 | C | ASN | D | 9 | 45.283 | 62.901 | 3.907 | 1.00 55.13 6 |
| | ATOM | 4999 | O | ASN | D | 9 | 46.175 | 62.117 | 3.593 | 1.00 54.15 8 |
| | ATOM | 5000 | N | ILE | D | 10 | 45.167 | 63.416 | 5.129 | 1.00 55.13 7 |
| | ATOM | 5001 | CA | ILE | D | 10 | 46.099 | 63.077 | 6.195 | 1.00 54.61 6 |
| 15 | ATOM | 5002 | CB | ILE | D | 10 | 45.660 | 63.693 | 7.534 | 1.00 54.44 6 |
| | ATOM | 5003 | CG2 | ILE | D | 10 | 46.585 | 63.218 | 8.651 | 1.00 53.71 6 |
| | ATOM | 5004 | CG1 | ILE | D | 10 | 45.683 | 65.222 | 7.435 | 1.00 52.93 6 |
| | ATOM | 5005 | CD1 | ILE | D | 10 | 45.083 | 65.916 | 8.605 | 1.00 47.92 6 |
| | ATOM | 5006 | C | ILE | D | 10 | 46.177 | 61.566 | 6.365 | 1.00 56.15 6 |
| 20 | ATOM | 5007 | O | ILE | D | 10 | 47.258 | 60.992 | 6.496 | 1.00 57.11 8 |
| | ATOM | 5008 | N | ARG | D | 11 | 45.018 | 60.927 | 6.363 | 1.00 56.48 7 |
| | ATOM | 5009 | CA | ARG | D | 11 | 44.938 | 59.494 | 6.512 | 1.00 58.41 6 |
| | ATOM | 5010 | CB | ARG | D | 11 | 43.478 | 59.070 | 6.428 | 1.00 63.58 6 |
| | ATOM | 5011 | CG | ARG | D | 11 | 43.229 | 57.585 | 6.631 | 1.00 70.33 6 |
| 25 | ATOM | 5012 | CD | ARG | D | 11 | 43.398 | 57.219 | 8.100 | 1.00 79.03 6 |
| | ATOM | 5013 | NE | ARG | D | 11 | 42.703 | 55.980 | 8.448 | 1.00 85.37 7 |
| | ATOM | 5014 | CZ | ARG | D | 11 | 41.466 | 55.685 | 8.037 | 1.00 88.61 6 |
| | ATOM | 5015 | NH1 | ARG | D | 11 | 40.795 | 56.548 | 7.249 | 1.00 89.11 7 |
| | ATOM | 5016 | NH2 | ARG | D | 11 | 40.890 | 54.545 | 8.434 | 1.00 87.93 7 |
| 30 | ATOM | 5017 | C | ARG | D | 11 | 45.721 | 58.778 | 5.425 | 1.00 58.93 6 |
| | ATOM | 5018 | O | ARG | D | 11 | 46.497 | 57.862 | 5.698 | 1.00 58.85 8 |
| | ATOM | 5019 | N | GLN | D | 12 | 45.507 | 59.211 | 4.186 | 1.00 59.05 7 |
| | ATOM | 5020 | CA | GLN | D | 12 | 46.131 | 58.596 | 3.024 | 1.00 57.95 6 |
| | ATOM | 5021 | CB | GLN | D | 12 | 45.345 | 58.958 | 1.780 | 1.00 57.48 6 |
| 35 | ATOM | 5022 | CG | GLN | D | 12 | 44.961 | 57.767 | 0.955 | 1.00 61.67 6 |
| | ATOM | 5023 | CD | GLN | D | 12 | 43.773 | 57.069 | 1.525 | 1.00 61.71 6 |
| | ATOM | 5024 | OE1 | GLN | D | 12 | 42.729 | 57.685 | 1.698 | 1.00 64.71 8 |
| | ATOM | 5025 | NE2 | GLN | D | 12 | 43.912 | 55.784 | 1.831 | 1.00 59.81 7 |
| | ATOM | 5026 | C | GLN | D | 12 | 47.589 | 58.926 | 2.769 | 1.00 57.99 6 |
| 40 | ATOM | 5027 | O | GLN | D | 12 | 48.280 | 58.169 | 2.097 | 1.00 58.62 8 |
| | ATOM | 5028 | N | THR | D | 13 | 48.070 | 60.046 | 3.291 | 1.00 57.97 7 |
| | ATOM | 5029 | CA | THR | D | 13 | 49.452 | 60.433 | 3.042 | 1.00 58.22 6 |
| | ATOM | 5030 | CB | THR | D | 13 | 49.520 | 61.855 | 2.464 | 1.00 56.90 6 |
| | ATOM | 5031 | OG1 | THR | D | 13 | 48.907 | 62.774 | 3.377 | 1.00 53.15 8 |
| 45 | ATOM | 5032 | CG2 | THR | D | 13 | 48.808 | 61.923 | 1.110 | 1.00 56.04 6 |
| | ATOM | 5033 | C | THR | D | 13 | 50.361 | 60.394 | 4.255 | 1.00 60.59 6 |
| | ATOM | 5034 | O | THR | D | 13 | 51.589 | 60.416 | 4.120 | 1.00 61.33 8 |
| | ATOM | 5035 | N | SER | D | 14 | 49.762 | 60.335 | 5.440 | 1.00 61.87 7 |
| | ATOM | 5036 | CA | SER | D | 14 | 50.542 | 60.332 | 6.669 | 1.00 61.93 6 |
| 50 | ATOM | 5037 | CB | SER | D | 14 | 49.634 | 60.613 | 7.863 | 1.00 61.53 6 |
| | ATOM | 5038 | OG | SER | D | 14 | 50.417 | 60.962 | 8.988 | 1.00 62.76 8 |
| | ATOM | 5039 | C | SER | D | 14 | 51.323 | 59.035 | 6.903 | 1.00 61.38 6 |
| | ATOM | 5040 | O | SER | D | 14 | 50.922 | 57.950 | 6.467 | 1.00 62.07 8 |
| | ATOM | 5041 | N | ARG | D | 15 | 52.444 | 59.175 | 7.596 | 1.00 59.21 7 |
| 55 | ATOM | 5042 | CA | ARG | D | 15 | 53.317 | 58.061 | 7.911 | 1.00 58.97 6 |
| | ATOM | 5043 | CB | ARG | D | 15 | 54.553 | 58.087 | 7.011 | 1.00 59.72 6 |
| | ATOM | 5044 | CG | ARG | D | 15 | 54.219 | 57.978 | 5.528 | 1.00 62.38 6 |
| | ATOM | 5045 | CD | ARG | D | 15 | 55.455 | 57.608 | 4.738 | 1.00 63.96 6 |
| | ATOM | 5046 | NE | ARG | D | 15 | 56.013 | 56.364 | 5.254 | 1.00 66.53 7 |
| 60 | ATOM | 5047 | CZ | ARG | D | 15 | 57.207 | 55.873 | 4.929 | 1.00 66.36 6 |
| | ATOM | 5048 | NH1 | ARG | D | 15 | 57.985 | 56.528 | 4.080 | 1.00 65.36 7 |
| | ATOM | 5049 | NH2 | ARG | D | 15 | 57.623 | 54.721 | 5.457 | 1.00 67.99 7 |
| | ATOM | 5050 | C | ARG | D | 15 | 53.724 | 58.182 | 9.376 | 1.00 57.69 6 |
| | ATOM | 5051 | O | ARG | D | 15 | 54.705 | 58.859 | 9.715 | 1.00 57.96 8 |
| | ATOM | 5052 | N | PRO | D | 16 | 52.967 | 57.517 | 10.265 | 1.00 55.24 7 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 5053 | CD | PRO | D | 16 | 51.785 | 56.700 | 9.935 | 1.00 | 51.06 | 6 |
| | ATOM | 5054 | CA | PRO | D | 16 | 53.200 | 57.524 | 11.709 | 1.00 | 51.86 | 6 |
| | ATOM | 5055 | CB | PRO | D | 16 | 52.104 | 56.602 | 12.236 | 1.00 | 49.85 | 6 |
| | ATOM | 5056 | CG | PRO | D | 16 | 51.031 | 56.720 | 11.226 | 1.00 | 51.02 | 6 |
| 5 | ATOM | 5057 | C | PRO | D | 16 | 54.580 | 57.066 | 12.130 | 1.00 | 49.97 | 6 |
| | ATOM | 5058 | O | PRO | D | 16 | 55.034 | 57.387 | 13.220 | 1.00 | 48.83 | 8 |
| | ATOM | 5059 | N | ASP | D | 17 | 55.247 | 56.313 | 11.270 | 1.00 | 50.05 | 7 |
| | ATOM | 5060 | CA | ASP | D | 17 | 56.568 | 55.809 | 11.612 | 1.00 | 53.82 | 6 |
| | ATOM | 5061 | CB | ASP | D | 17 | 56.796 | 54.419 | 10.981 | 1.00 | 57.43 | 6 |
| 10 | ATOM | 5062 | CG | ASP | D | 17 | 55.979 | 53.320 | 11.666 | 1.00 | 63.55 | 6 |
| | ATOM | 5063 | OD1 | ASP | D | 17 | 55.728 | 53.431 | 12.892 | 1.00 | 63.43 | 8 |
| | ATOM | 5064 | OD2 | ASP | D | 17 | 55.598 | 52.330 | 10.985 | 1.00 | 66.47 | 8 |
| | ATOM | 5065 | C | ASP | D | 17 | 57.710 | 56.733 | 11.218 | 1.00 | 52.72 | 6 |
| | ATOM | 5066 | O | ASP | D | 17 | 58.875 | 56.406 | 11.440 | 1.00 | 54.00 | 8 |
| 15 | ATOM | 5067 | N | VAL | D | 18 | 57.384 | 57.888 | 10.653 | 1.00 | 50.54 | 7 |
| | ATOM | 5068 | CA | VAL | D | 18 | 58.418 | 58.808 | 10.209 | 1.00 | 51.72 | 6 |
| | ATOM | 5069 | CB | VAL | D | 18 | 58.353 | 58.992 | 8.680 | 1.00 | 52.70 | 6 |
| | ATOM | 5070 | CG1 | VAL | D | 18 | 59.487 | 59.869 | 8.209 | 1.00 | 52.67 | 6 |
| | ATOM | 5071 | CG2 | VAL | D | 18 | 58.426 | 57.642 | 7.998 | 1.00 | 53.16 | 6 |
| 20 | ATOM | 5072 | C | VAL | D | 18 | 58.402 | 60.181 | 10.865 | 1.00 | 51.90 | 6 |
| | ATOM | 5073 | O | VAL | D | 18 | 57.463 | 60.955 | 10.716 | 1.00 | 50.79 | 8 |
| | ATOM | 5074 | N | ILE | D | 19 | 59.475 | 60.473 | 11.586 | 1.00 | 52.81 | 7 |
| | ATOM | 5075 | CA | ILE | D | 19 | 59.646 | 61.748 | 12.280 | 1.00 | 54.09 | 6 |
| | ATOM | 5076 | CB | ILE | D | 19 | 60.960 | 61.699 | 13.116 | 1.00 | 53.08 | 6 |
| 25 | ATOM | 5077 | CG2 | ILE | D | 19 | 62.168 | 61.565 | 12.194 | 1.00 | 53.31 | 6 |
| | ATOM | 5078 | CG1 | ILE | D | 19 | 61.074 | 62.919 | 14.027 | 1.00 | 52.13 | 6 |
| | ATOM | 5079 | CD1 | ILE | D | 19 | 62.157 | 62.753 | 15.086 | 1.00 | 49.47 | 6 |
| | ATOM | 5080 | C | ILE | D | 19 | 59.675 | 62.907 | 11.255 | 1.00 | 56.58 | 6 |
| | ATOM | 5081 | O | ILE | D | 19 | 60.436 | 62.877 | 10.274 | 1.00 | 57.79 | 8 |
| 30 | ATOM | 5082 | N | PRO | D | 20 | 58.833 | 63.936 | 11.464 | 1.00 | 56.89 | 7 |
| | ATOM | 5083 | CD | PRO | D | 20 | 57.915 | 64.059 | 12.603 | 1.00 | 56.43 | 6 |
| | ATOM | 5084 | CA | PRO | D | 20 | 58.725 | 65.113 | 10.587 | 1.00 | 58.17 | 6 |
| | ATOM | 5085 | CB | PRO | D | 20 | 57.505 | 65.856 | 11.148 | 1.00 | 57.33 | 6 |
| | ATOM | 5086 | CG | PRO | D | 20 | 56.812 | 64.848 | 12.009 | 1.00 | 56.81 | 6 |
| 35 | ATOM | 5087 | C | PRO | D | 20 | 59.985 | 66.004 | 10.585 | 1.00 | 60.38 | 6 |
| | ATOM | 5088 | O | PRO | D | 20 | 59.920 | 67.215 | 10.802 | 1.00 | 57.93 | 8 |
| | ATOM | 5089 | N | THR | D | 21 | 61.128 | 65.391 | 10.329 | 1.00 | 64.41 | 7 |
| | ATOM | 5090 | CA | THR | D | 21 | 62.392 | 66.106 | 10.320 | 1.00 | 68.99 | 6 |
| | ATOM | 5091 | CB | THR | D | 21 | 63.546 | 65.121 | 10.552 | 1.00 | 68.83 | 6 |
| 40 | ATOM | 5092 | OG1 | THR | D | 21 | 63.899 | 65.152 | 11.939 | 1.00 | 69.74 | 8 |
| | ATOM | 5093 | CG2 | THR | D | 21 | 64.760 | 65.457 | 9.688 | 1.00 | 69.49 | 6 |
| | ATOM | 5094 | C | THR | D | 21 | 62.671 | 66.926 | 9.067 | 1.00 | 73.81 | 6 |
| | ATOM | 5095 | O | THR | D | 21 | 62.480 | 66.457 | 7.936 | 1.00 | 75.27 | 8 |
| | ATOM | 5096 | N | GLN | D | 22 | 63.130 | 68.157 | 9.285 | 1.00 | 77.41 | 7 |
| 45 | ATOM | 5097 | CA | GLN | D | 22 | 63.481 | 69.076 | 8.203 | 1.00 | 81.17 | 6 |
| | ATOM | 5098 | CB | GLN | D | 22 | 62.791 | 70.416 | 8.428 | 1.00 | 82.19 | 6 |
| | ATOM | 5099 | CG | GLN | D | 22 | 61.281 | 70.306 | 8.543 | 1.00 | 84.72 | 6 |
| | ATOM | 5100 | CD | GLN | D | 22 | 60.689 | 71.416 | 9.409 | 1.00 | 86.15 | 6 |
| | ATOM | 5101 | OE1 | GLN | D | 22 | 60.939 | 71.471 | 10.623 | 1.00 | 85.03 | 8 |
| 50 | ATOM | 5102 | NE2 | GLN | D | 22 | 59.901 | 72.309 | 8.789 | 1.00 | 86.55 | 7 |
| | ATOM | 5103 | C | GLN | D | 22 | 65.001 | 69.262 | 8.233 | 1.00 | 83.27 | 6 |
| | ATOM | 5104 | O | GLN | D | 22 | 65.538 | 69.912 | 9.147 | 1.00 | 83.34 | 8 |
| | ATOM | 5105 | N | ARG | D | 23 | 65.691 | 68.686 | 7.243 | 1.00 | 85.66 | 7 |
| | ATOM | 5106 | CA | ARG | D | 23 | 67.159 | 68.767 | 7.170 | 1.00 | 87.34 | 6 |
| 55 | ATOM | 5107 | CB | ARG | D | 23 | 67.625 | 70.231 | 7.105 | 1.00 | 88.19 | 6 |
| | ATOM | 5108 | CG | ARG | D | 23 | 67.453 | 70.875 | 5.742 | 1.00 | 89.83 | 6 |
| | ATOM | 5109 | CD | ARG | D | 23 | 66.246 | 71.822 | 5.674 | 1.00 | 92.72 | 6 |
| | ATOM | 5110 | NE | ARG | D | 23 | 65.994 | 72.293 | 4.298 | 1.00 | 95.59 | 7 |
| | ATOM | 5111 | CZ | ARG | D | 23 | 66.904 | 72.868 | 3.497 | 1.00 | 95.46 | 6 |
| 60 | ATOM | 5112 | NH1 | ARG | D | 23 | 68.158 | 73.068 | 3.914 | 1.00 | 93.60 | 7 |
| | ATOM | 5113 | NH2 | ARG | D | 23 | 66.555 | 73.226 | 2.257 | 1.00 | 94.84 | 7 |

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|----|------|------|-----|----------|--------|--------|--------|------|---------|
| 5 | ATOM | 5114 | C | ARG D 23 | 67.768 | 68.079 | 8.399 | 1.00 | 87.43 6 |
| | ATOM | 5115 | O | ARG D 23 | 67.201 | 67.105 | 8.907 | 1.00 | 88.35 8 |
| | ATOM | 5116 | N | ASP D 24 | 68.912 | 68.570 | 8.875 | 1.00 | 87.68 7 |
| | ATOM | 5117 | CA | ASP D 24 | 69.538 | 67.975 | 10.055 | 1.00 | 86.96 6 |
| | ATOM | 5118 | CB | ASP D 24 | 71.041 | 68.283 | 10.123 | 1.00 | 91.11 6 |
| 10 | ATOM | 5119 | CG | ASP D 24 | 71.627 | 68.719 | 8.780 | 1.00 | 94.40 6 |
| | ATOM | 5120 | OD1 | ASP D 24 | 71.599 | 67.908 | 7.806 | 1.00 | 95.87 8 |
| | ATOM | 5121 | OD2 | ASP D 24 | 72.121 | 69.881 | 8.712 | 1.00 | 95.25 8 |
| | ATOM | 5122 | C | ASP D 24 | 68.864 | 68.594 | 11.274 | 1.00 | 85.02 6 |
| | ATOM | 5123 | O | ASP D 24 | 69.279 | 68.347 | 12.414 | 1.00 | 83.40 8 |
| 15 | ATOM | 5124 | N | ARG D 25 | 67.836 | 69.409 | 11.026 | 1.00 | 82.95 7 |
| | ATOM | 5125 | CA | ARG D 25 | 67.112 | 70.062 | 12.111 | 1.00 | 81.58 6 |
| | ATOM | 5126 | CB | ARG D 25 | 66.218 | 71.189 | 11.585 | 1.00 | 83.67 6 |
| | ATOM | 5127 | CG | ARG D 25 | 66.951 | 72.455 | 11.150 | 1.00 | 88.52 6 |
| | ATOM | 5128 | CD | ARG D 25 | 65.941 | 73.597 | 10.942 | 1.00 | 92.65 6 |
| 20 | ATOM | 5129 | NE | ARG D 25 | 66.579 | 74.866 | 10.584 | 1.00 | 96.29 7 |
| | ATOM | 5130 | CZ | ARG D 25 | 65.928 | 76.024 | 10.463 | 1.00 | 98.03 6 |
| | ATOM | 5131 | NH1 | ARG D 25 | 64.608 | 76.073 | 10.673 | 1.00 | 98.35 7 |
| | ATOM | 5132 | NH2 | ARG D 25 | 66.597 | 77.136 | 10.142 | 1.00 | 98.69 7 |
| | ATOM | 5133 | C | ARG D 25 | 66.241 | 69.091 | 12.901 | 1.00 | 78.66 6 |
| 25 | ATOM | 5134 | O | ARG D 25 | 65.480 | 68.303 | 12.325 | 1.00 | 79.51 8 |
| | ATOM | 5135 | N | PRO D 26 | 66.353 | 69.127 | 14.237 | 1.00 | 74.94 7 |
| | ATOM | 5136 | CD | PRO D 26 | 67.383 | 69.831 | 15.020 | 1.00 | 73.76 6 |
| | ATOM | 5137 | CA | PRO D 26 | 65.562 | 68.252 | 15.101 | 1.00 | 71.13 6 |
| | ATOM | 5138 | CB | PRO D 26 | 66.202 | 68.450 | 16.483 | 1.00 | 71.49 6 |
| 30 | ATOM | 5139 | CG | PRO D 26 | 67.608 | 68.884 | 16.165 | 1.00 | 72.18 6 |
| | ATOM | 5140 | C | PRO D 26 | 64.115 | 68.738 | 15.095 | 1.00 | 67.33 6 |
| | ATOM | 5141 | O | PRO D 26 | 63.834 | 69.874 | 14.713 | 1.00 | 65.48 8 |
| | ATOM | 5142 | N | VAL D 27 | 63.198 | 67.870 | 15.510 | 1.00 | 63.87 7 |
| | ATOM | 5143 | CA | VAL D 27 | 61.806 | 68.258 | 15.596 | 1.00 | 58.65 6 |
| 35 | ATOM | 5144 | CB | VAL D 27 | 60.849 | 67.036 | 15.494 | 1.00 | 57.16 6 |
| | ATOM | 5145 | CG1 | VAL D 27 | 59.462 | 67.401 | 15.998 | 1.00 | 54.11 6 |
| | ATOM | 5146 | CG2 | VAL D 27 | 60.755 | 66.579 | 14.052 | 1.00 | 56.19 6 |
| | ATOM | 5147 | C | VAL D 27 | 61.705 | 68.896 | 16.968 | 1.00 | 56.92 6 |
| | ATOM | 5148 | O | VAL D 27 | 62.164 | 68.337 | 17.961 | 1.00 | 55.97 8 |
| 40 | ATOM | 5149 | N | ALA D 28 | 61.136 | 70.088 | 17.019 | 1.00 | 56.42 7 |
| | ATOM | 5150 | CA | ALA D 28 | 60.999 | 70.767 | 18.287 | 1.00 | 55.56 6 |
| | ATOM | 5151 | CB | ALA D 28 | 61.057 | 72.269 | 18.095 | 1.00 | 55.33 6 |
| | ATOM | 5152 | C | ALA D 28 | 59.688 | 70.371 | 18.923 | 1.00 | 54.28 6 |
| | ATOM | 5153 | O | ALA D 28 | 58.617 | 70.741 | 18.440 | 1.00 | 54.43 8 |
| 45 | ATOM | 5154 | N | VAL D 29 | 59.800 | 69.603 | 20.006 | 1.00 | 52.62 7 |
| | ATOM | 5155 | CA | VAL D 29 | 58.657 | 69.127 | 20.775 | 1.00 | 50.60 6 |
| | ATOM | 5156 | CB | VAL D 29 | 58.715 | 67.599 | 21.016 | 1.00 | 48.93 6 |
| | ATOM | 5157 | CG1 | VAL D 29 | 57.543 | 67.162 | 21.871 | 1.00 | 46.20 6 |
| | ATOM | 5158 | CG2 | VAL D 29 | 58.718 | 66.868 | 19.692 | 1.00 | 47.60 6 |
| 50 | ATOM | 5159 | C | VAL D 29 | 58.652 | 69.805 | 22.131 | 1.00 | 50.77 6 |
| | ATOM | 5160 | O | VAL D 29 | 59.657 | 69.806 | 22.852 | 1.00 | 51.59 8 |
| | ATOM | 5161 | N | SER D 30 | 57.517 | 70.395 | 22.471 | 1.00 | 50.31 7 |
| | ATOM | 5162 | CA | SER D 30 | 57.373 | 71.049 | 23.754 | 1.00 | 52.56 6 |
| | ATOM | 5163 | CB | SER D 30 | 56.794 | 72.449 | 23.575 | 1.00 | 53.44 6 |
| 55 | ATOM | 5164 | OG | SER D 30 | 55.514 | 72.393 | 22.966 | 1.00 | 56.80 8 |
| | ATOM | 5165 | C | SER D 30 | 56.442 | 70.188 | 24.598 | 1.00 | 53.29 6 |
| | ATOM | 5166 | O | SER D 30 | 55.397 | 69.746 | 24.126 | 1.00 | 55.20 8 |
| | ATOM | 5167 | N | VAL D 31 | 56.845 | 69.947 | 25.841 | 1.00 | 54.04 7 |
| | ATOM | 5168 | CA | VAL D 31 | 56.089 | 69.130 | 26.780 | 1.00 | 56.25 6 |
| 60 | ATOM | 5169 | CB | VAL D 31 | 56.911 | 67.898 | 27.241 | 1.00 | 58.16 6 |
| | ATOM | 5170 | CG1 | VAL D 31 | 56.015 | 66.914 | 27.986 | 1.00 | 56.17 6 |
| | ATOM | 5171 | CG2 | VAL D 31 | 57.573 | 67.234 | 26.043 | 1.00 | 58.28 6 |
| | ATOM | 5172 | C | VAL D 31 | 55.753 | 69.947 | 28.015 | 1.00 | 57.41 6 |
| | ATOM | 5173 | O | VAL D 31 | 56.607 | 70.632 | 28.570 | 1.00 | 58.01 8 |
| | ATOM | 5174 | N | SER D 32 | 54.508 | 69.850 | 28.458 | 1.00 | 59.19 7 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 5175 | CA | SER | D | 32 | 54.062 | 70.594 | 29.628 | 1.00 | 59.47 | 6 |
| | ATOM | 5176 | CB | SER | D | 32 | 53.467 | 71.934 | 29.175 | 1.00 | 60.04 | 6 |
| | ATOM | 5177 | OG | SER | D | 32 | 52.892 | 72.641 | 30.256 | 1.00 | 62.30 | 8 |
| | ATOM | 5178 | C | SER | D | 32 | 53.023 | 69.799 | 30.433 | 1.00 | 58.78 | 6 |
| 5 | ATOM | 5179 | O | SER | D | 32 | 51.906 | 69.572 | 29.966 | 1.00 | 59.54 | 8 |
| | ATOM | 5180 | N | LEU | D | 33 | 53.390 | 69.379 | 31.638 | 1.00 | 56.81 | 7 |
| | ATOM | 5181 | CA | LEU | D | 33 | 52.468 | 68.629 | 32.472 | 1.00 | 56.85 | 6 |
| | ATOM | 5182 | CB | LEU | D | 33 | 53.217 | 67.702 | 33.426 | 1.00 | 54.23 | 6 |
| | ATOM | 5183 | CG | LEU | D | 33 | 54.192 | 66.726 | 32.775 | 1.00 | 55.08 | 6 |
| 10 | ATOM | 5184 | CD1 | LEU | D | 33 | 54.665 | 65.709 | 33.818 | 1.00 | 53.15 | 6 |
| | ATOM | 5185 | CD2 | LEU | D | 33 | 53.513 | 66.034 | 31.614 | 1.00 | 54.80 | 6 |
| | ATOM | 5186 | C | LEU | D | 33 | 51.623 | 69.572 | 33.291 | 1.00 | 56.91 | 6 |
| | ATOM | 5187 | O | LEU | D | 33 | 52.136 | 70.542 | 33.829 | 1.00 | 59.29 | 8 |
| | ATOM | 5188 | N | LYS | D | 34 | 50.327 | 69.294 | 33.366 | 1.00 | 56.10 | 7 |
| 15 | ATOM | 5189 | CA | LYS | D | 34 | 49.422 | 70.089 | 34.171 | 1.00 | 55.13 | 6 |
| | ATOM | 5190 | CB | LYS | D | 34 | 48.311 | 70.694 | 33.320 | 1.00 | 58.38 | 6 |
| | ATOM | 5191 | CG | LYS | D | 34 | 48.802 | 71.519 | 32.146 | 1.00 | 65.52 | 6 |
| | ATOM | 5192 | CD | LYS | D | 34 | 49.581 | 72.764 | 32.581 | 1.00 | 69.06 | 6 |
| | ATOM | 5193 | CE | LYS | D | 34 | 50.100 | 73.559 | 31.364 | 1.00 | 72.37 | 6 |
| 20 | ATOM | 5194 | NZ | LYS | D | 34 | 50.855 | 74.801 | 31.747 | 1.00 | 72.05 | 7 |
| | ATOM | 5195 | C | LYS | D | 34 | 48.838 | 69.065 | 35.118 | 1.00 | 53.80 | 6 |
| | ATOM | 5196 | O | LYS | D | 34 | 48.123 | 68.167 | 34.685 | 1.00 | 55.04 | 8 |
| | ATOM | 5197 | N | PHE | D | 35 | 49.144 | 69.173 | 36.405 | 1.00 | 51.60 | 7 |
| | ATOM | 5198 | CA | PHE | D | 35 | 48.616 | 68.200 | 37.346 | 1.00 | 49.19 | 6 |
| 25 | ATOM | 5199 | CB | PHE | D | 35 | 49.441 | 68.199 | 38.616 | 1.00 | 46.49 | 6 |
| | ATOM | 5200 | CG | PHE | D | 35 | 50.838 | 67.733 | 38.393 | 1.00 | 48.31 | 6 |
| | ATOM | 5201 | CD1 | PHE | D | 35 | 51.823 | 68.617 | 37.964 | 1.00 | 46.94 | 6 |
| | ATOM | 5202 | CD2 | PHE | D | 35 | 51.159 | 66.387 | 38.530 | 1.00 | 49.16 | 6 |
| | ATOM | 5203 | CE1 | PHE | D | 35 | 53.109 | 68.170 | 37.668 | 1.00 | 48.04 | 6 |
| 30 | ATOM | 5204 | CE2 | PHE | D | 35 | 52.449 | 65.925 | 38.235 | 1.00 | 50.28 | 6 |
| | ATOM | 5205 | CZ | PHE | D | 35 | 53.424 | 66.818 | 37.802 | 1.00 | 48.13 | 6 |
| | ATOM | 5206 | C | PHE | D | 35 | 47.136 | 68.352 | 37.642 | 1.00 | 49.07 | 6 |
| | ATOM | 5207 | O | PHE | D | 35 | 46.626 | 69.449 | 37.869 | 1.00 | 49.57 | 8 |
| | ATOM | 5208 | N | ILE | D | 36 | 46.451 | 67.217 | 37.600 | 1.00 | 47.68 | 7 |
| 35 | ATOM | 5209 | CA | ILE | D | 36 | 45.030 | 67.156 | 37.827 | 1.00 | 44.72 | 6 |
| | ATOM | 5210 | CB | ILE | D | 36 | 44.352 | 66.334 | 36.731 | 1.00 | 43.48 | 6 |
| | ATOM | 5211 | CG2 | ILE | D | 36 | 42.850 | 66.369 | 36.914 | 1.00 | 41.45 | 6 |
| | ATOM | 5212 | CG1 | ILE | D | 36 | 44.752 | 66.877 | 35.360 | 1.00 | 43.86 | 6 |
| | ATOM | 5213 | CD1 | ILE | D | 36 | 44.398 | 68.324 | 35.152 | 1.00 | 46.64 | 6 |
| 40 | ATOM | 5214 | C | ILE | D | 36 | 44.719 | 66.525 | 39.164 | 1.00 | 44.81 | 6 |
| | ATOM | 5215 | O | ILE | D | 36 | 43.677 | 66.798 | 39.743 | 1.00 | 46.51 | 8 |
| | ATOM | 5216 | N | ASN | D | 37 | 45.612 | 65.678 | 39.661 | 1.00 | 42.08 | 7 |
| | ATOM | 5217 | CA | ASN | D | 37 | 45.363 | 65.030 | 40.939 | 1.00 | 42.31 | 6 |
| | ATOM | 5218 | CB | ASN | D | 37 | 44.117 | 64.140 | 40.834 | 1.00 | 41.66 | 6 |
| 45 | ATOM | 5219 | CG | ASN | D | 37 | 43.392 | 63.990 | 42.159 | 1.00 | 43.88 | 6 |
| | ATOM | 5220 | OD1 | ASN | D | 37 | 44.015 | 63.785 | 43.200 | 1.00 | 43.62 | 8 |
| | ATOM | 5221 | ND2 | ASN | D | 37 | 42.068 | 64.085 | 42.124 | 1.00 | 38.41 | 7 |
| | ATOM | 5222 | C | ASN | D | 37 | 46.539 | 64.186 | 41.426 | 1.00 | 43.81 | 6 |
| | ATOM | 5223 | O | ASN | D | 37 | 47.380 | 63.752 | 40.640 | 1.00 | 40.93 | 8 |
| 50 | ATOM | 5224 | N | ILE | D | 38 | 46.588 | 63.977 | 42.740 | 1.00 | 43.93 | 7 |
| | ATOM | 5225 | CA | ILE | D | 38 | 47.612 | 63.163 | 43.372 | 1.00 | 44.58 | 6 |
| | ATOM | 5226 | CB | ILE | D | 38 | 48.496 | 64.013 | 44.246 | 1.00 | 42.93 | 6 |
| | ATOM | 5227 | CG2 | ILE | D | 38 | 49.473 | 63.140 | 44.989 | 1.00 | 39.88 | 6 |
| | ATOM | 5228 | CG1 | ILE | D | 38 | 49.220 | 65.028 | 43.359 | 1.00 | 43.19 | 6 |
| 55 | ATOM | 5229 | CD1 | ILE | D | 38 | 49.944 | 66.110 | 44.084 | 1.00 | 44.94 | 6 |
| | ATOM | 5230 | C | ILE | D | 38 | 46.795 | 62.183 | 44.190 | 1.00 | 47.97 | 6 |
| | ATOM | 5231 | O | ILE | D | 38 | 46.169 | 62.565 | 45.162 | 1.00 | 50.60 | 8 |
| | ATOM | 5232 | N | LEU | D | 39 | 46.802 | 60.916 | 43.777 | 1.00 | 50.68 | 7 |
| | ATOM | 5233 | CA | LEU | D | 39 | 45.979 | 59.874 | 44.388 | 1.00 | 51.24 | 6 |
| 60 | ATOM | 5234 | CB | LEU | D | 39 | 45.489 | 58.944 | 43.287 | 1.00 | 51.95 | 6 |
| | ATOM | 5235 | CG | LEU | D | 39 | 44.834 | 59.723 | 42.141 | 1.00 | 54.64 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 5236 | CD1 | LEU | D | 39 | 44.356 | 58.777 | 41.068 | 1.00 | 53.53 | 6 |
| | ATOM | 5237 | CD2 | LEU | D | 39 | 43.666 | 60.542 | 42.696 | 1.00 | 53.70 | 6 |
| | ATOM | 5238 | C | LEU | D | 39 | 46.520 | 59.041 | 45.529 | 1.00 | 53.82 | 6 |
| | ATOM | 5239 | O | LEU | D | 39 | 45.793 | 58.750 | 46.479 | 1.00 | 54.77 | 8 |
| 5 | ATOM | 5240 | N | GLU | D | 40 | 47.771 | 58.620 | 45.437 | 1.00 | 54.21 | 7 |
| | ATOM | 5241 | CA | GLU | D | 40 | 48.349 | 57.825 | 46.507 | 1.00 | 56.24 | 6 |
| | ATOM | 5242 | CB | GLU | D | 40 | 48.278 | 56.339 | 46.204 | 1.00 | 58.19 | 6 |
| | ATOM | 5243 | CG | GLU | D | 40 | 46.873 | 55.801 | 46.103 | 1.00 | 65.00 | 6 |
| | ATOM | 5244 | CD | GLU | D | 40 | 46.844 | 54.291 | 45.938 | 1.00 | 68.23 | 6 |
| 10 | ATOM | 5245 | OE1 | GLU | D | 40 | 47.443 | 53.791 | 44.955 | 1.00 | 70.63 | 8 |
| | ATOM | 5246 | OE2 | GLU | D | 40 | 46.226 | 53.611 | 46.789 | 1.00 | 68.96 | 8 |
| | ATOM | 5247 | C | GLU | D | 40 | 49.785 | 58.198 | 46.702 | 1.00 | 56.38 | 6 |
| | ATOM | 5248 | O | GLU | D | 40 | 50.541 | 58.355 | 45.746 | 1.00 | 59.25 | 8 |
| | ATOM | 5249 | N | VAL | D | 41 | 50.162 | 58.343 | 47.955 | 1.00 | 55.49 | 7 |
| 15 | ATOM | 5250 | CA | VAL | D | 41 | 51.517 | 58.695 | 48.273 | 1.00 | 54.71 | 6 |
| | ATOM | 5251 | CB | VAL | D | 41 | 51.590 | 60.145 | 48.811 | 1.00 | 55.08 | 6 |
| | ATOM | 5252 | CG1 | VAL | D | 41 | 52.954 | 60.431 | 49.361 | 1.00 | 55.65 | 6 |
| | ATOM | 5253 | CG2 | VAL | D | 41 | 51.273 | 61.125 | 47.696 | 1.00 | 55.07 | 6 |
| | ATOM | 5254 | C | VAL | D | 41 | 52.003 | 57.713 | 49.309 | 1.00 | 54.17 | 6 |
| 20 | ATOM | 5255 | O | VAL | D | 41 | 51.232 | 57.239 | 50.136 | 1.00 | 53.51 | 8 |
| | ATOM | 5256 | N | ASN | D | 42 | 53.280 | 57.381 | 49.233 | 1.00 | 54.90 | 7 |
| | ATOM | 5257 | CA | ASN | D | 42 | 53.880 | 56.473 | 50.182 | 1.00 | 56.47 | 6 |
| | ATOM | 5258 | CB | ASN | D | 42 | 53.944 | 55.056 | 49.612 | 1.00 | 55.97 | 6 |
| | ATOM | 5259 | CG | ASN | D | 42 | 54.306 | 54.025 | 50.661 | 1.00 | 56.38 | 6 |
| 25 | ATOM | 5260 | OD1 | ASN | D | 42 | 55.272 | 54.191 | 51.408 | 1.00 | 55.15 | 8 |
| | ATOM | 5261 | ND2 | ASN | D | 42 | 53.536 | 52.947 | 50.717 | 1.00 | 56.12 | 7 |
| | ATOM | 5262 | C | ASN | D | 42 | 55.278 | 57.022 | 50.420 | 1.00 | 58.56 | 6 |
| | ATOM | 5263 | O | ASN | D | 42 | 56.154 | 56.912 | 49.567 | 1.00 | 58.83 | 8 |
| | ATOM | 5264 | N | GLU | D | 43 | 55.474 | 57.639 | 51.579 | 1.00 | 59.69 | 7 |
| 30 | ATOM | 5265 | CA | GLU | D | 43 | 56.771 | 58.208 | 51.905 | 1.00 | 60.97 | 6 |
| | ATOM | 5266 | CB | GLU | D | 43 | 56.640 | 59.192 | 53.065 | 1.00 | 63.50 | 6 |
| | ATOM | 5267 | CG | GLU | D | 43 | 57.921 | 59.959 | 53.341 | 1.00 | 67.19 | 6 |
| | ATOM | 5268 | CD | GLU | D | 43 | 57.725 | 61.121 | 54.303 | 1.00 | 68.84 | 6 |
| | ATOM | 5269 | OE1 | GLU | D | 43 | 58.743 | 61.734 | 54.682 | 1.00 | 70.83 | 8 |
| 35 | ATOM | 5270 | OE2 | GLU | D | 43 | 56.568 | 61.427 | 54.670 | 1.00 | 67.80 | 8 |
| | ATOM | 5271 | C | GLU | D | 43 | 57.792 | 57.134 | 52.246 | 1.00 | 59.80 | 6 |
| | ATOM | 5272 | O | GLU | D | 43 | 58.993 | 57.356 | 52.138 | 1.00 | 59.85 | 8 |
| | ATOM | 5273 | N | ILE | D | 44 | 57.301 | 55.969 | 52.653 | 1.00 | 59.27 | 7 |
| | ATOM | 5274 | CA | ILE | D | 44 | 58.164 | 54.858 | 53.006 | 1.00 | 59.05 | 6 |
| 40 | ATOM | 5275 | CB | ILE | D | 44 | 57.373 | 53.723 | 53.681 | 1.00 | 59.62 | 6 |
| | ATOM | 5276 | CG2 | ILE | D | 44 | 58.300 | 52.527 | 53.945 | 1.00 | 59.50 | 6 |
| | ATOM | 5277 | CG1 | ILE | D | 44 | 56.752 | 54.217 | 54.982 | 1.00 | 58.87 | 6 |
| | ATOM | 5278 | CD1 | ILE | D | 44 | 57.768 | 54.484 | 56.073 | 1.00 | 60.45 | 6 |
| | ATOM | 5279 | C | ILE | D | 44 | 58.801 | 54.286 | 51.751 | 1.00 | 59.04 | 6 |
| 45 | ATOM | 5280 | O | ILE | D | 44 | 60.001 | 54.029 | 51.723 | 1.00 | 60.06 | 8 |
| | ATOM | 5281 | N | THR | D | 45 | 57.986 | 54.080 | 50.719 | 1.00 | 57.12 | 7 |
| | ATOM | 5282 | CA | THR | D | 45 | 58.461 | 53.513 | 49.464 | 1.00 | 54.05 | 6 |
| | ATOM | 5283 | CB | THR | D | 45 | 57.410 | 52.576 | 48.857 | 1.00 | 52.43 | 6 |
| | ATOM | 5284 | OG1 | THR | D | 45 | 56.204 | 53.304 | 48.628 | 1.00 | 49.39 | 8 |
| 50 | ATOM | 5285 | CG2 | THR | D | 45 | 57.128 | 51.426 | 49.788 | 1.00 | 49.70 | 6 |
| | ATOM | 5286 | C | THR | D | 45 | 58.833 | 54.551 | 48.417 | 1.00 | 53.32 | 6 |
| | ATOM | 5287 | O | THR | D | 45 | 59.427 | 54.215 | 47.397 | 1.00 | 56.15 | 8 |
| | ATOM | 5288 | N | ASN | D | 46 | 58.493 | 55.809 | 48.666 | 1.00 | 51.82 | 7 |
| | ATOM | 5289 | CA | ASN | D | 46 | 58.796 | 56.874 | 47.723 | 1.00 | 51.33 | 6 |
| 55 | ATOM | 5290 | CB | ASN | D | 46 | 60.305 | 57.022 | 47.567 | 1.00 | 51.66 | 6 |
| | ATOM | 5291 | CG | ASN | D | 46 | 60.874 | 58.117 | 48.434 | 1.00 | 52.73 | 6 |
| | ATOM | 5292 | OD1 | ASN | D | 46 | 62.057 | 58.105 | 48.765 | 1.00 | 52.55 | 8 |
| | ATOM | 5293 | ND2 | ASN | D | 46 | 60.041 | 59.078 | 48.793 | 1.00 | 50.90 | 7 |
| | ATOM | 5294 | C | ASN | D | 46 | 58.156 | 56.618 | 46.360 | 1.00 | 50.97 | 6 |
| 60 | ATOM | 5295 | O | ASN | D | 46 | 58.820 | 56.668 | 45.325 | 1.00 | 53.17 | 8 |
| | ATOM | 5296 | N | GLU | D | 47 | 56.858 | 56.348 | 46.371 | 1.00 | 48.99 | 7 |

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|----|------|------|-----|-----|------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 5297 | CA | GLU | D 47 | 56.118 | 56.091 | 45.155 | 1.00 | 48.91 | 6 |
| | ATOM | 5298 | CB | GLU | D 47 | 55.717 | 54.627 | 45.105 | 1.00 | 46.66 | 6 |
| | ATOM | 5299 | CG | GLU | D 47 | 56.888 | 53.678 | 45.006 | 1.00 | 47.02 | 6 |
| | ATOM | 5300 | CD | GLU | D 47 | 56.458 | 52.227 | 45.018 | 1.00 | 49.64 | 6 |
| | ATOM | 5301 | OE1 | GLU | D 47 | 55.302 | 51.956 | 44.644 | 1.00 | 48.30 | 8 |
| 10 | ATOM | 5302 | OE2 | GLU | D 47 | 57.276 | 51.357 | 45.391 | 1.00 | 51.88 | 8 |
| | ATOM | 5303 | C | GLU | D 47 | 54.888 | 56.992 | 45.111 | 1.00 | 50.12 | 6 |
| | ATOM | 5304 | O | GLU | D 47 | 54.222 | 57.202 | 46.125 | 1.00 | 50.30 | 8 |
| | ATOM | 5305 | N | VAL | D 48 | 54.591 | 57.531 | 43.936 | 1.00 | 50.20 | 7 |
| | ATOM | 5306 | CA | VAL | D 48 | 53.455 | 58.423 | 43.793 | 1.00 | 52.05 | 6 |
| 15 | ATOM | 5307 | CB | VAL | D 48 | 53.925 | 59.861 | 43.502 | 1.00 | 53.36 | 6 |
| | ATOM | 5308 | CG1 | VAL | D 48 | 52.727 | 60.778 | 43.352 | 1.00 | 56.39 | 6 |
| | ATOM | 5309 | CG2 | VAL | D 48 | 54.801 | 60.352 | 44.620 | 1.00 | 54.18 | 6 |
| | ATOM | 5310 | C | VAL | D 48 | 52.522 | 57.995 | 42.673 | 1.00 | 51.50 | 6 |
| | ATOM | 5311 | O | VAL | D 48 | 52.962 | 57.552 | 41.617 | 1.00 | 53.49 | 8 |
| 20 | ATOM | 5312 | N | ASP | D 49 | 51.231 | 58.137 | 42.910 | 1.00 | 49.46 | 7 |
| | ATOM | 5313 | CA | ASP | D 49 | 50.241 | 57.777 | 41.920 | 1.00 | 49.81 | 6 |
| | ATOM | 5314 | CB | ASP | D 49 | 49.241 | 56.813 | 42.535 | 1.00 | 52.06 | 6 |
| | ATOM | 5315 | CG | ASP | D 49 | 48.447 | 56.086 | 41.508 | 1.00 | 53.16 | 6 |
| | ATOM | 5316 | OD1 | ASP | D 49 | 48.086 | 56.719 | 40.499 | 1.00 | 53.36 | 8 |
| 25 | ATOM | 5317 | OD2 | ASP | D 49 | 48.176 | 54.887 | 41.717 | 1.00 | 57.15 | 8 |
| | ATOM | 5318 | C | ASP | D 49 | 49.583 | 59.105 | 41.580 | 1.00 | 49.01 | 6 |
| | ATOM | 5319 | O | ASP | D 49 | 48.818 | 59.646 | 42.373 | 1.00 | 48.57 | 8 |
| | ATOM | 5320 | N | VAL | D 50 | 49.882 | 59.624 | 40.394 | 1.00 | 48.09 | 7 |
| | ATOM | 5321 | CA | VAL | D 50 | 49.380 | 60.928 | 39.986 | 1.00 | 47.49 | 6 |
| 30 | ATOM | 5322 | CB | VAL | D 50 | 50.561 | 61.946 | 39.980 | 1.00 | 49.68 | 6 |
| | ATOM | 5323 | CG1 | VAL | D 50 | 51.428 | 61.732 | 38.761 | 1.00 | 49.68 | 6 |
| | ATOM | 5324 | CG2 | VAL | D 50 | 50.048 | 63.356 | 40.017 | 1.00 | 54.48 | 6 |
| | ATOM | 5325 | C | VAL | D 50 | 48.671 | 60.966 | 38.630 | 1.00 | 44.84 | 6 |
| | ATOM | 5326 | O | VAL | D 50 | 48.885 | 60.107 | 37.791 | 1.00 | 46.99 | 8 |
| 35 | ATOM | 5327 | N | VAL | D 51 | 47.816 | 61.971 | 38.443 | 1.00 | 41.91 | 7 |
| | ATOM | 5328 | CA | VAL | D 51 | 47.067 | 62.186 | 37.204 | 1.00 | 40.48 | 6 |
| | ATOM | 5329 | CB | VAL | D 51 | 45.560 | 62.225 | 37.460 | 1.00 | 37.45 | 6 |
| | ATOM | 5330 | CG1 | VAL | D 51 | 44.837 | 62.697 | 36.213 | 1.00 | 39.17 | 6 |
| | ATOM | 5331 | CG2 | VAL | D 51 | 45.070 | 60.860 | 37.859 | 1.00 | 36.64 | 6 |
| 40 | ATOM | 5332 | C | VAL | D 51 | 47.479 | 63.538 | 36.628 | 1.00 | 42.16 | 6 |
| | ATOM | 5333 | O | VAL | D 51 | 47.560 | 64.508 | 37.359 | 1.00 | 46.47 | 8 |
| | ATOM | 5334 | N | PHE | D 52 | 47.726 | 63.617 | 35.328 | 1.00 | 40.72 | 7 |
| | ATOM | 5335 | CA | PHE | D 52 | 48.144 | 64.877 | 34.738 | 1.00 | 42.11 | 6 |
| | ATOM | 5336 | CB | PHE | D 52 | 49.635 | 65.072 | 34.984 | 1.00 | 41.64 | 6 |
| 45 | ATOM | 5337 | CG | PHE | D 52 | 50.491 | 64.007 | 34.362 | 1.00 | 42.87 | 6 |
| | ATOM | 5338 | CD1 | PHE | D 52 | 50.887 | 64.099 | 33.038 | 1.00 | 44.21 | 6 |
| | ATOM | 5339 | CD2 | PHE | D 52 | 50.868 | 62.891 | 35.088 | 1.00 | 42.70 | 6 |
| | ATOM | 5340 | CE1 | PHE | D 52 | 51.642 | 63.100 | 32.447 | 1.00 | 42.06 | 6 |
| | ATOM | 5341 | CE2 | PHE | D 52 | 51.624 | 61.886 | 34.506 | 1.00 | 42.93 | 6 |
| 50 | ATOM | 5342 | CZ | PHE | D 52 | 52.010 | 61.990 | 33.185 | 1.00 | 41.42 | 6 |
| | ATOM | 5343 | C | PHE | D 52 | 47.870 | 64.940 | 33.241 | 1.00 | 44.00 | 6 |
| | ATOM | 5344 | O | PHE | D 52 | 47.606 | 63.931 | 32.610 | 1.00 | 46.55 | 8 |
| | ATOM | 5345 | N | TRP | D 53 | 47.934 | 66.133 | 32.673 | 1.00 | 43.89 | 7 |
| | ATOM | 5346 | CA | TRP | D 53 | 47.726 | 66.294 | 31.253 | 1.00 | 44.08 | 6 |
| 55 | ATOM | 5347 | CB | TRP | D 53 | 46.919 | 67.538 | 30.948 | 1.00 | 45.09 | 6 |
| | ATOM | 5348 | CG | TRP | D 53 | 45.537 | 67.474 | 31.396 | 1.00 | 46.86 | 6 |
| | ATOM | 5349 | CD2 | TRP | D 53 | 44.596 | 68.542 | 31.383 | 1.00 | 49.97 | 6 |
| | ATOM | 5350 | CE2 | TRP | D 53 | 43.372 | 68.024 | 31.855 | 1.00 | 50.77 | 6 |
| | ATOM | 5351 | CE3 | TRP | D 53 | 44.666 | 69.891 | 31.017 | 1.00 | 52.22 | 6 |
| 60 | ATOM | 5352 | CD1 | TRP | D 53 | 44.877 | 66.383 | 31.863 | 1.00 | 47.58 | 6 |
| | ATOM | 5353 | NE1 | TRP | D 53 | 43.571 | 66.700 | 32.141 | 1.00 | 48.69 | 7 |
| | ATOM | 5354 | CZ2 | TRP | D 53 | 42.222 | 68.808 | 31.973 | 1.00 | 52.23 | 6 |
| | ATOM | 5355 | CZ3 | TRP | D 53 | 43.521 | 70.672 | 31.135 | 1.00 | 54.33 | 6 |
| | ATOM | 5356 | CH2 | TRP | D 53 | 42.313 | 70.126 | 31.610 | 1.00 | 53.10 | 6 |
| | ATOM | 5357 | C | TRP | D 53 | 49.085 | 66.452 | 30.640 | 1.00 | 46.17 | 6 |

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|----|------|------|-----|----------|--------|--------|--------|------|---------|
| 5 | ATOM | 5358 | O | TRP D 53 | 49.803 | 67.384 | 30.960 | 1.00 | 46.13 8 |
| | ATOM | 5359 | N | GLN D 54 | 49.444 | 65.532 | 29.760 | 1.00 | 49.02 7 |
| | ATOM | 5360 | CA | GLN D 54 | 50.741 | 65.592 | 29.112 | 1.00 | 48.49 6 |
| | ATOM | 5361 | CB | GLN D 54 | 51.248 | 64.184 | 28.809 | 1.00 | 48.38 6 |
| | ATOM | 5362 | CG | GLN D 54 | 52.677 | 64.135 | 28.317 | 1.00 | 50.78 6 |
| 10 | ATOM | 5363 | CD | GLN D 54 | 53.339 | 62.792 | 28.583 | 1.00 | 52.08 6 |
| | ATOM | 5364 | OE1 | GLN D 54 | 53.409 | 62.336 | 29.721 | 1.00 | 52.24 8 |
| | ATOM | 5365 | NE2 | GLN D 54 | 53.832 | 62.158 | 27.532 | 1.00 | 53.79 7 |
| | ATOM | 5366 | C | GLN D 54 | 50.560 | 66.408 | 27.849 | 1.00 | 49.01 6 |
| | ATOM | 5367 | O | GLN D 54 | 50.504 | 65.892 | 26.735 | 1.00 | 48.80 8 |
| 15 | ATOM | 5368 | N | GLN D 55 | 50.441 | 67.708 | 28.058 | 1.00 | 51.39 7 |
| | ATOM | 5369 | CA | GLN D 55 | 50.256 | 68.665 | 26.985 | 1.00 | 53.26 6 |
| | ATOM | 5370 | CB | GLN D 55 | 49.964 | 70.022 | 27.609 | 1.00 | 56.68 6 |
| | ATOM | 5371 | CG | GLN D 55 | 49.913 | 71.176 | 26.652 | 1.00 | 66.24 6 |
| | ATOM | 5372 | CD | GLN D 55 | 49.355 | 72.406 | 27.326 | 1.00 | 70.72 6 |
| 20 | ATOM | 5373 | OE1 | GLN D 55 | 49.611 | 72.637 | 28.525 | 1.00 | 72.96 8 |
| | ATOM | 5374 | NE2 | GLN D 55 | 48.584 | 73.210 | 26.573 | 1.00 | 70.76 7 |
| | ATOM | 5375 | C | GLN D 55 | 51.494 | 68.697 | 26.092 | 1.00 | 51.66 6 |
| | ATOM | 5376 | O | GLN D 55 | 52.533 | 69.249 | 26.457 | 1.00 | 52.73 8 |
| | ATOM | 5377 | N | THR D 56 | 51.373 | 68.091 | 24.920 | 1.00 | 48.75 7 |
| 25 | ATOM | 5378 | CA | THR D 56 | 52.485 | 68.005 | 23.988 | 1.00 | 48.81 6 |
| | ATOM | 5379 | CB | THR D 56 | 52.769 | 66.534 | 23.617 | 1.00 | 48.35 6 |
| | ATOM | 5380 | OG1 | THR D 56 | 52.793 | 65.733 | 24.801 | 1.00 | 50.12 8 |
| | ATOM | 5381 | CG2 | THR D 56 | 54.101 | 66.408 | 22.925 | 1.00 | 47.54 6 |
| | ATOM | 5382 | C | THR D 56 | 52.198 | 68.771 | 22.709 | 1.00 | 48.92 6 |
| 30 | ATOM | 5383 | O | THR D 56 | 51.051 | 68.862 | 22.275 | 1.00 | 50.82 8 |
| | ATOM | 5384 | N | THR D 57 | 53.243 | 69.320 | 22.101 | 1.00 | 48.36 7 |
| | ATOM | 5385 | CA | THR D 57 | 53.080 | 70.069 | 20.860 | 1.00 | 47.70 6 |
| | ATOM | 5386 | CB | THR D 57 | 52.766 | 71.563 | 21.126 | 1.00 | 47.89 6 |
| | ATOM | 5387 | OG1 | THR D 57 | 51.521 | 71.679 | 21.834 | 1.00 | 48.44 8 |
| 35 | ATOM | 5388 | CG2 | THR D 57 | 52.642 | 72.317 | 19.826 | 1.00 | 47.29 6 |
| | ATOM | 5389 | C | THR D 57 | 54.322 | 69.988 | 19.995 | 1.00 | 47.52 6 |
| | ATOM | 5390 | O | THR D 57 | 55.446 | 69.954 | 20.496 | 1.00 | 48.40 8 |
| | ATOM | 5391 | N | TRP D 58 | 54.113 | 69.928 | 18.686 | 1.00 | 46.65 7 |
| | ATOM | 5392 | CA | TRP D 58 | 55.221 | 69.883 | 17.749 | 1.00 | 45.92 6 |
| 40 | ATOM | 5393 | CB | TRP D 58 | 55.890 | 68.501 | 17.750 | 1.00 | 46.07 6 |
| | ATOM | 5394 | CG | TRP D 58 | 55.055 | 67.379 | 17.192 | 1.00 | 46.21 6 |
| | ATOM | 5395 | CD2 | TRP D 58 | 54.099 | 66.585 | 17.904 | 1.00 | 45.21 6 |
| | ATOM | 5396 | CE2 | TRP D 58 | 53.517 | 65.702 | 16.976 | 1.00 | 45.14 6 |
| | ATOM | 5397 | CE3 | TRP D 58 | 53.675 | 66.537 | 19.240 | 1.00 | 44.92 6 |
| 45 | ATOM | 5398 | CD1 | TRP D 58 | 55.018 | 66.952 | 15.902 | 1.00 | 44.73 6 |
| | ATOM | 5399 | NE1 | TRP D 58 | 54.097 | 65.945 | 15.761 | 1.00 | 46.01 7 |
| | ATOM | 5400 | CZ2 | TRP D 58 | 52.533 | 64.783 | 17.336 | 1.00 | 46.24 6 |
| | ATOM | 5401 | CZ3 | TRP D 58 | 52.696 | 65.618 | 19.596 | 1.00 | 45.62 6 |
| | ATOM | 5402 | CH2 | TRP D 58 | 52.138 | 64.755 | 18.646 | 1.00 | 45.70 6 |
| 50 | ATOM | 5403 | C | TRP D 58 | 54.679 | 70.236 | 16.386 | 1.00 | 47.55 6 |
| | ATOM | 5404 | O | TRP D 58 | 53.494 | 70.509 | 16.237 | 1.00 | 46.55 8 |
| | ATOM | 5405 | N | SER D 59 | 55.537 | 70.226 | 15.381 | 1.00 | 51.25 7 |
| | ATOM | 5406 | CA | SER D 59 | 55.097 | 70.602 | 14.051 | 1.00 | 54.98 6 |
| | ATOM | 5407 | CB | SER D 59 | 55.688 | 71.974 | 13.705 | 1.00 | 56.59 6 |
| 55 | ATOM | 5408 | OG | SER D 59 | 54.969 | 72.610 | 12.659 | 1.00 | 61.93 8 |
| | ATOM | 5409 | C | SER D 59 | 55.457 | 69.592 | 12.967 | 1.00 | 55.53 6 |
| | ATOM | 5410 | O | SER D 59 | 56.587 | 69.119 | 12.889 | 1.00 | 54.93 8 |
| | ATOM | 5411 | N | ASP D 60 | 54.479 | 69.279 | 12.126 | 1.00 | 57.49 7 |
| | ATOM | 5412 | CA | ASP D 60 | 54.660 | 68.338 | 11.028 | 1.00 | 59.17 6 |
| 60 | ATOM | 5413 | CB | ASP D 60 | 53.898 | 67.046 | 11.316 | 1.00 | 61.53 6 |
| | ATOM | 5414 | CG | ASP D 60 | 54.141 | 65.967 | 10.275 | 1.00 | 63.57 6 |
| | ATOM | 5415 | OD1 | ASP D 60 | 54.465 | 66.300 | 9.120 | 1.00 | 64.52 8 |
| | ATOM | 5416 | OD2 | ASP D 60 | 53.988 | 64.773 | 10.611 | 1.00 | 64.89 8 |
| | ATOM | 5417 | C | ASP D 60 | 54.067 | 69.020 | 9.811 | 1.00 | 60.52 6 |
| | ATOM | 5418 | O | ASP D 60 | 52.847 | 69.016 | 9.615 | 1.00 | 59.95 8 |

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|----|------|------|-----|-----|---|------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 5419 | N | ARG | D | 61 | 54.937 | 69.609 | 8.995 | 1.00 | 62.50 | 7 |
| | ATOM | 5420 | CA | ARG | D | 61 | 54.503 | 70.334 | 7.800 | 1.00 | 64.61 | 6 |
| | ATOM | 5421 | CB | ARG | D | 61 | 55.672 | 71.137 | 7.205 | 1.00 | 67.57 | 6 |
| | ATOM | 5422 | CG | ARG | D | 61 | 56.000 | 72.468 | 7.909 | 1.00 | 73.40 | 6 |
| | ATOM | 5423 | CD | ARG | D | 61 | 56.968 | 73.283 | 7.037 | 1.00 | 81.08 | 6 |
| 10 | ATOM | 5424 | NE | ARG | D | 61 | 57.268 | 74.635 | 7.537 | 1.00 | 86.56 | 7 |
| | ATOM | 5425 | CZ | ARG | D | 61 | 58.057 | 75.522 | 6.910 | 1.00 | 87.41 | 6 |
| | ATOM | 5426 | NH1 | ARG | D | 61 | 58.642 | 75.210 | 5.749 | 1.00 | 87.01 | 7 |
| | ATOM | 5427 | NH2 | ARG | D | 61 | 58.246 | 76.731 | 7.433 | 1.00 | 87.16 | 7 |
| | ATOM | 5428 | C | ARG | D | 61 | 53.867 | 69.476 | 6.703 | 1.00 | 64.15 | 6 |
| 15 | ATOM | 5429 | O | ARG | D | 61 | 53.145 | 69.998 | 5.844 | 1.00 | 63.51 | 8 |
| | ATOM | 5430 | N | THR | D | 62 | 54.121 | 68.170 | 6.722 | 1.00 | 62.13 | 7 |
| | ATOM | 5431 | CA | THR | D | 62 | 53.542 | 67.303 | 5.704 | 1.00 | 61.28 | 6 |
| | ATOM | 5432 | CB | THR | D | 62 | 54.171 | 65.886 | 5.716 | 1.00 | 62.74 | 6 |
| | ATOM | 5433 | OG1 | THR | D | 62 | 53.809 | 65.201 | 6.924 | 1.00 | 65.20 | 8 |
| 20 | ATOM | 5434 | CG2 | THR | D | 62 | 55.692 | 65.974 | 5.624 | 1.00 | 63.05 | 6 |
| | ATOM | 5435 | C | THR | D | 62 | 52.030 | 67.184 | 5.911 | 1.00 | 60.41 | 6 |
| | ATOM | 5436 | O | THR | D | 62 | 51.313 | 66.619 | 5.073 | 1.00 | 60.16 | 8 |
| | ATOM | 5437 | N | LEU | D | 63 | 51.551 | 67.731 | 7.025 | 1.00 | 59.01 | 7 |
| | ATOM | 5438 | CA | LEU | D | 63 | 50.124 | 67.705 | 7.356 | 1.00 | 57.25 | 6 |
| 25 | ATOM | 5439 | CB | LEU | D | 63 | 49.932 | 67.483 | 8.860 | 1.00 | 55.13 | 6 |
| | ATOM | 5440 | CG | LEU | D | 63 | 50.567 | 66.242 | 9.489 | 1.00 | 54.37 | 6 |
| | ATOM | 5441 | CD1 | LEU | D | 63 | 50.396 | 66.277 | 10.997 | 1.00 | 51.58 | 6 |
| | ATOM | 5442 | CD2 | LEU | D | 63 | 49.917 | 65.002 | 8.903 | 1.00 | 55.32 | 6 |
| | ATOM | 5443 | C | LEU | D | 63 | 49.446 | 69.017 | 6.973 | 1.00 | 56.83 | 6 |
| 30 | ATOM | 5444 | O | LEU | D | 63 | 48.228 | 69.091 | 6.904 | 1.00 | 55.62 | 8 |
| | ATOM | 5445 | N | ALA | D | 64 | 50.241 | 70.052 | 6.730 | 1.00 | 56.52 | 7 |
| | ATOM | 5446 | CA | ALA | D | 64 | 49.702 | 71.362 | 6.388 | 1.00 | 56.94 | 6 |
| | ATOM | 5447 | CB | ALA | D | 64 | 50.843 | 72.351 | 6.196 | 1.00 | 56.75 | 6 |
| | ATOM | 5448 | C | ALA | D | 64 | 48.825 | 71.336 | 5.147 | 1.00 | 57.08 | 6 |
| 35 | ATOM | 5449 | O | ALA | D | 64 | 49.091 | 70.571 | 4.222 | 1.00 | 59.16 | 8 |
| | ATOM | 5450 | N | TRP | D | 65 | 47.785 | 72.174 | 5.138 | 1.00 | 56.39 | 7 |
| | ATOM | 5451 | CA | TRP | D | 65 | 46.853 | 72.286 | 4.008 | 1.00 | 57.81 | 6 |
| | ATOM | 5452 | CB | TRP | D | 65 | 45.718 | 71.279 | 4.183 | 1.00 | 52.06 | 6 |
| | ATOM | 5453 | CG | TRP | D | 65 | 44.662 | 71.708 | 5.139 | 1.00 | 49.69 | 6 |
| 40 | ATOM | 5454 | CD2 | TRP | D | 65 | 44.574 | 71.383 | 6.532 | 1.00 | 48.62 | 6 |
| | ATOM | 5455 | CE2 | TRP | D | 65 | 43.386 | 71.974 | 7.027 | 1.00 | 50.58 | 6 |
| | ATOM | 5456 | CE3 | TRP | D | 65 | 45.379 | 70.649 | 7.409 | 1.00 | 45.78 | 6 |
| | ATOM | 5457 | CD1 | TRP | D | 65 | 43.563 | 72.466 | 4.855 | 1.00 | 51.37 | 6 |
| | ATOM | 5458 | NE1 | TRP | D | 65 | 42.787 | 72.631 | 5.985 | 1.00 | 51.62 | 7 |
| 45 | ATOM | 5459 | CZ2 | TRP | D | 65 | 42.987 | 71.849 | 8.358 | 1.00 | 48.81 | 6 |
| | ATOM | 5460 | CZ3 | TRP | D | 65 | 44.983 | 70.525 | 8.731 | 1.00 | 45.33 | 6 |
| | ATOM | 5461 | CH2 | TRP | D | 65 | 43.797 | 71.122 | 9.193 | 1.00 | 48.88 | 6 |
| | ATOM | 5462 | C | TRP | D | 65 | 46.281 | 73.723 | 3.873 | 1.00 | 60.73 | 6 |
| | ATOM | 5463 | O | TRP | D | 65 | 46.309 | 74.493 | 4.839 | 1.00 | 61.78 | 8 |
| 50 | ATOM | 5464 | N | ASN | D | 66 | 45.757 | 74.081 | 2.692 | 1.00 | 63.62 | 7 |
| | ATOM | 5465 | CA | ASN | D | 66 | 45.198 | 75.423 | 2.474 | 1.00 | 66.29 | 6 |
| | ATOM | 5466 | CB | ASN | D | 66 | 44.996 | 75.702 | 0.975 | 1.00 | 67.13 | 6 |
| | ATOM | 5467 | CG | ASN | D | 66 | 44.462 | 77.129 | 0.700 | 1.00 | 70.42 | 6 |
| | ATOM | 5468 | OD1 | ASN | D | 66 | 44.317 | 77.560 | -0.465 | 1.00 | 68.84 | 8 |
| 55 | ATOM | 5469 | ND2 | ASN | D | 66 | 44.167 | 77.866 | 1.780 | 1.00 | 71.49 | 7 |
| | ATOM | 5470 | C | ASN | D | 66 | 43.886 | 75.676 | 3.221 | 1.00 | 67.74 | 6 |
| | ATOM | 5471 | O | ASN | D | 66 | 42.823 | 75.208 | 2.820 | 1.00 | 67.77 | 8 |
| | ATOM | 5472 | N | SER | D | 67 | 43.982 | 76.466 | 4.289 | 1.00 | 70.41 | 7 |
| | ATOM | 5473 | CA | SER | D | 67 | 42.852 | 76.810 | 5.156 | 1.00 | 72.51 | 6 |
| 60 | ATOM | 5474 | CB | SER | D | 67 | 43.363 | 77.028 | 6.586 | 1.00 | 71.50 | 6 |
| | ATOM | 5475 | OG | SER | D | 67 | 42.519 | 77.911 | 7.324 | 1.00 | 70.60 | 8 |
| | ATOM | 5476 | C | SER | D | 67 | 42.021 | 78.025 | 4.763 | 1.00 | 74.90 | 6 |
| | ATOM | 5477 | O | SER | D | 67 | 41.148 | 78.434 | 5.530 | 1.00 | 75.98 | 8 |
| | ATOM | 5478 | N | SER | D | 68 | 42.272 | 78.603 | 3.589 | 1.00 | 77.57 | 7 |
| | ATOM | 5479 | CA | SER | D | 68 | 41.538 | 79.805 | 3.157 | 1.00 | 79.08 | 6 |

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|----|------|------|-----|-------|----|--------|--------|--------|------|-------|---|
| | ATOM | 5480 | CB | SER D | 68 | 41.991 | 80.243 | 1.761 | 1.00 | 78.86 | 6 |
| | ATOM | 5481 | OG | SER D | 68 | 41.612 | 79.297 | 0.776 | 1.00 | 79.93 | 8 |
| | ATOM | 5482 | C | SER D | 68 | 40.012 | 79.707 | 3.157 | 1.00 | 80.32 | 6 |
| | ATOM | 5483 | O | SER D | 68 | 39.328 | 80.655 | 3.552 | 1.00 | 81.34 | 8 |
| 5 | ATOM | 5484 | N | HIS D | 69 | 39.471 | 78.578 | 2.711 | 1.00 | 80.85 | 7 |
| | ATOM | 5485 | CA | HIS D | 69 | 38.027 | 78.421 | 2.663 | 1.00 | 81.81 | 6 |
| | ATOM | 5486 | CB | HIS D | 69 | 37.562 | 78.625 | 1.239 | 1.00 | 84.77 | 6 |
| | ATOM | 5487 | CG | HIS D | 69 | 37.857 | 79.994 | 0.729 | 1.00 | 88.72 | 6 |
| | ATOM | 5488 | CD2 | HIS D | 69 | 38.776 | 80.436 | -0.166 | 1.00 | 89.11 | 6 |
| 10 | ATOM | 5489 | ND1 | HIS D | 69 | 37.226 | 81.117 | 1.227 | 1.00 | 88.96 | 7 |
| | ATOM | 5490 | CE1 | HIS D | 69 | 37.748 | 82.193 | 0.660 | 1.00 | 90.17 | 6 |
| | ATOM | 5491 | NE2 | HIS D | 69 | 38.691 | 81.809 | -0.188 | 1.00 | 89.66 | 7 |
| | ATOM | 5492 | C | HIS D | 69 | 37.607 | 77.066 | 3.176 | 1.00 | 81.57 | 6 |
| | ATOM | 5493 | O | HIS D | 69 | 36.624 | 76.459 | 2.713 | 1.00 | 80.65 | 8 |
| 15 | ATOM | 5494 | N | SER D | 70 | 38.362 | 76.606 | 4.162 | 1.00 | 80.66 | 7 |
| | ATOM | 5495 | CA | SER D | 70 | 38.110 | 75.319 | 4.770 | 1.00 | 79.33 | 6 |
| | ATOM | 5496 | CB | SER D | 70 | 38.813 | 74.240 | 3.941 | 1.00 | 79.59 | 6 |
| | ATOM | 5497 | OG | SER D | 70 | 40.110 | 74.675 | 3.550 | 1.00 | 79.40 | 8 |
| | ATOM | 5498 | C | SER D | 70 | 38.624 | 75.348 | 6.211 | 1.00 | 77.66 | 6 |
| 20 | ATOM | 5499 | O | SER D | 70 | 39.520 | 76.135 | 6.545 | 1.00 | 76.61 | 8 |
| | ATOM | 5500 | N | PRO D | 71 | 38.037 | 74.514 | 7.088 | 1.00 | 76.20 | 7 |
| | ATOM | 5501 | CD | PRO D | 71 | 36.862 | 73.660 | 6.801 | 1.00 | 76.18 | 6 |
| | ATOM | 5502 | CA | PRO D | 71 | 38.420 | 74.425 | 8.502 | 1.00 | 74.80 | 6 |
| | ATOM | 5503 | CB | PRO D | 71 | 37.788 | 73.101 | 8.935 | 1.00 | 75.09 | 6 |
| 25 | ATOM | 5504 | CG | PRO D | 71 | 36.454 | 73.145 | 8.196 | 1.00 | 75.33 | 6 |
| | ATOM | 5505 | C | PRO D | 71 | 39.933 | 74.465 | 8.704 | 1.00 | 73.25 | 6 |
| | ATOM | 5506 | O | PRO D | 71 | 40.685 | 73.855 | 7.939 | 1.00 | 73.92 | 8 |
| | ATOM | 5507 | N | ASP D | 72 | 40.369 | 75.180 | 9.738 | 1.00 | 71.15 | 7 |
| | ATOM | 5508 | CA | ASP D | 72 | 41.794 | 75.329 | 10.033 | 1.00 | 69.88 | 6 |
| 30 | ATOM | 5509 | CB | ASP D | 72 | 42.077 | 76.680 | 10.721 | 1.00 | 74.59 | 6 |
| | ATOM | 5510 | CG | ASP D | 72 | 40.874 | 77.647 | 10.691 | 1.00 | 79.11 | 6 |
| | ATOM | 5511 | OD1 | ASP D | 72 | 41.131 | 78.882 | 10.737 | 1.00 | 79.05 | 8 |
| | ATOM | 5512 | OD2 | ASP D | 72 | 39.692 | 77.190 | 10.635 | 1.00 | 80.55 | 8 |
| | ATOM | 5513 | C | ASP D | 72 | 42.330 | 74.212 | 10.923 | 1.00 | 67.26 | 6 |
| 35 | ATOM | 5514 | O | ASP D | 72 | 43.540 | 73.973 | 10.975 | 1.00 | 66.51 | 8 |
| | ATOM | 5515 | N | GLN D | 73 | 41.421 | 73.556 | 11.637 | 1.00 | 63.43 | 7 |
| | ATOM | 5516 | CA | GLN D | 73 | 41.756 | 72.462 | 12.539 | 1.00 | 60.99 | 6 |
| | ATOM | 5517 | CB | GLN D | 73 | 41.653 | 72.909 | 13.981 | 1.00 | 63.13 | 6 |
| | ATOM | 5518 | CG | GLN D | 73 | 42.774 | 73.723 | 14.533 | 1.00 | 65.58 | 6 |
| 40 | ATOM | 5519 | CD | GLN D | 73 | 42.460 | 74.099 | 15.957 | 1.00 | 67.92 | 6 |
| | ATOM | 5520 | OE1 | GLN D | 73 | 41.413 | 74.692 | 16.216 | 1.00 | 70.47 | 8 |
| | ATOM | 5521 | NE2 | GLN D | 73 | 43.338 | 73.737 | 16.895 | 1.00 | 69.20 | 7 |
| | ATOM | 5522 | C | GLN D | 73 | 40.810 | 71.287 | 12.397 | 1.00 | 58.94 | 6 |
| | ATOM | 5523 | O | GLN D | 73 | 39.639 | 71.445 | 12.029 | 1.00 | 59.19 | 8 |
| 45 | ATOM | 5524 | N | VAL D | 74 | 41.317 | 70.108 | 12.737 | 1.00 | 56.36 | 7 |
| | ATOM | 5525 | CA | VAL D | 74 | 40.531 | 68.883 | 12.698 | 1.00 | 52.71 | 6 |
| | ATOM | 5526 | CB | VAL D | 74 | 40.635 | 68.177 | 11.329 | 1.00 | 51.38 | 6 |
| | ATOM | 5527 | CG1 | VAL D | 74 | 39.944 | 68.998 | 10.260 | 1.00 | 48.73 | 6 |
| | ATOM | 5528 | CG2 | VAL D | 74 | 42.087 | 67.951 | 10.973 | 1.00 | 48.36 | 6 |
| 50 | ATOM | 5529 | C | VAL D | 74 | 41.089 | 67.959 | 13.760 | 1.00 | 50.70 | 6 |
| | ATOM | 5530 | O | VAL D | 74 | 42.240 | 68.108 | 14.173 | 1.00 | 49.32 | 8 |
| | ATOM | 5531 | N | SER D | 75 | 40.264 | 67.023 | 14.215 | 1.00 | 48.60 | 7 |
| | ATOM | 5532 | CA | SER D | 75 | 40.696 | 66.051 | 15.206 | 1.00 | 46.92 | 6 |
| 55 | ATOM | 5533 | CB | SER D | 75 | 39.555 | 65.729 | 16.166 | 1.00 | 48.45 | 6 |
| | ATOM | 5534 | OG | SER D | 75 | 39.444 | 66.718 | 17.168 | 1.00 | 48.28 | 8 |
| | ATOM | 5535 | C | SER D | 75 | 41.159 | 64.789 | 14.487 | 1.00 | 44.70 | 6 |
| | ATOM | 5536 | O | SER D | 75 | 40.397 | 64.143 | 13.781 | 1.00 | 43.70 | 8 |
| | ATOM | 5537 | N | VAL D | 76 | 42.424 | 64.449 | 14.675 | 1.00 | 44.00 | 7 |
| | ATOM | 5538 | CA | VAL D | 76 | 43.024 | 63.281 | 14.039 | 1.00 | 43.43 | 6 |
| 60 | ATOM | 5539 | CB | VAL D | 76 | 44.283 | 63.687 | 13.264 | 1.00 | 44.79 | 6 |
| | ATOM | 5540 | CG1 | VAL D | 76 | 44.891 | 62.486 | 12.604 | 1.00 | 43.63 | 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 5541 | CG2 | VAL | D | 76 | 43.943 | 64.746 | 12.241 | 1.00 | 42.10 | 6 |
| | ATOM | 5542 | C | VAL | D | 76 | 43.419 | 62.193 | 15.034 | 1.00 | 43.50 | 6 |
| | ATOM | 5543 | O | VAL | D | 76 | 44.004 | 62.472 | 16.078 | 1.00 | 45.44 | 8 |
| | ATOM | 5544 | N | PRO | D | 77 | 43.102 | 60.929 | 14.721 | 1.00 | 42.76 | 7 |
| 5 | ATOM | 5545 | CD | PRO | D | 77 | 42.235 | 60.402 | 13.656 | 1.00 | 41.52 | 6 |
| | ATOM | 5546 | CA | PRO | D | 77 | 43.472 | 59.865 | 15.650 | 1.00 | 41.41 | 6 |
| | ATOM | 5547 | CB | PRO | D | 77 | 42.856 | 58.628 | 15.009 | 1.00 | 42.36 | 6 |
| | ATOM | 5548 | CG | PRO | D | 77 | 41.674 | 59.168 | 14.296 | 1.00 | 40.67 | 6 |
| 10 | ATOM | 5549 | C | PRO | D | 77 | 44.985 | 59.774 | 15.749 | 1.00 | 40.15 | 6 |
| | ATOM | 5550 | O | PRO | D | 77 | 45.687 | 59.922 | 14.762 | 1.00 | 39.02 | 8 |
| | ATOM | 5551 | N | ILE | D | 78 | 45.474 | 59.537 | 16.954 | 1.00 | 41.66 | 7 |
| | ATOM | 5552 | CA | ILE | D | 78 | 46.899 | 59.421 | 17.217 | 1.00 | 42.23 | 6 |
| | ATOM | 5553 | CB | ILE | D | 78 | 47.113 | 59.019 | 18.687 | 1.00 | 43.04 | 6 |
| | ATOM | 5554 | CG2 | ILE | D | 78 | 48.495 | 58.518 | 18.924 | 1.00 | 45.01 | 6 |
| 15 | ATOM | 5555 | CG1 | ILE | D | 78 | 46.872 | 60.236 | 19.555 | 1.00 | 47.88 | 6 |
| | ATOM | 5556 | CD1 | ILE | D | 78 | 47.618 | 61.461 | 19.057 | 1.00 | 48.43 | 6 |
| | ATOM | 5557 | C | ILE | D | 78 | 47.591 | 58.432 | 16.299 | 1.00 | 42.53 | 6 |
| | ATOM | 5558 | O | ILE | D | 78 | 48.717 | 58.643 | 15.880 | 1.00 | 44.25 | 8 |
| 20 | ATOM | 5559 | N | SER | D | 79 | 46.891 | 57.358 | 15.979 | 1.00 | 43.93 | 7 |
| | ATOM | 5560 | CA | SER | D | 79 | 47.410 | 56.302 | 15.127 | 1.00 | 43.22 | 6 |
| | ATOM | 5561 | CB | SER | D | 79 | 46.457 | 55.110 | 15.185 | 1.00 | 42.69 | 6 |
| | ATOM | 5562 | OG | SER | D | 79 | 45.130 | 55.523 | 14.910 | 1.00 | 43.59 | 8 |
| | ATOM | 5563 | C | SER | D | 79 | 47.661 | 56.692 | 13.668 | 1.00 | 42.26 | 6 |
| | ATOM | 5564 | O | SER | D | 79 | 48.319 | 55.953 | 12.937 | 1.00 | 41.56 | 8 |
| 25 | ATOM | 5565 | N | SER | D | 80 | 47.138 | 57.835 | 13.243 | 1.00 | 39.86 | 7 |
| | ATOM | 5566 | CA | SER | D | 80 | 47.326 | 58.282 | 11.871 | 1.00 | 40.25 | 6 |
| | ATOM | 5567 | CB | SER | D | 80 | 46.026 | 58.840 | 11.307 | 1.00 | 40.77 | 6 |
| | ATOM | 5568 | OG | SER | D | 80 | 45.025 | 57.845 | 11.259 | 1.00 | 48.70 | 8 |
| | ATOM | 5569 | C | SER | D | 80 | 48.413 | 59.342 | 11.742 | 1.00 | 41.01 | 6 |
| 30 | ATOM | 5570 | O | SER | D | 80 | 48.658 | 59.842 | 10.655 | 1.00 | 41.05 | 8 |
| | ATOM | 5571 | N | LEU | D | 81 | 49.067 | 59.671 | 12.847 | 1.00 | 39.67 | 7 |
| | ATOM | 5572 | CA | LEU | D | 81 | 50.112 | 60.678 | 12.844 | 1.00 | 39.96 | 6 |
| | ATOM | 5573 | CB | LEU | D | 81 | 49.703 | 61.886 | 13.684 | 1.00 | 40.31 | 6 |
| | ATOM | 5574 | CG | LEU | D | 81 | 48.371 | 62.571 | 13.448 | 1.00 | 42.96 | 6 |
| 35 | ATOM | 5575 | CD1 | LEU | D | 81 | 48.019 | 63.429 | 14.638 | 1.00 | 41.75 | 6 |
| | ATOM | 5576 | CD2 | LEU | D | 81 | 48.454 | 63.382 | 12.191 | 1.00 | 44.21 | 6 |
| | ATOM | 5577 | C | LEU | D | 81 | 51.357 | 60.109 | 13.472 | 1.00 | 38.80 | 6 |
| | ATOM | 5578 | O | LEU | D | 81 | 51.303 | 59.077 | 14.119 | 1.00 | 39.28 | 8 |
| | ATOM | 5579 | N | TRP | D | 82 | 52.478 | 60.795 | 13.276 | 1.00 | 37.55 | 7 |
| 40 | ATOM | 5580 | CA | TRP | D | 82 | 53.726 | 60.398 | 13.891 | 1.00 | 36.02 | 6 |
| | ATOM | 5581 | CB | TRP | D | 82 | 54.927 | 60.981 | 13.158 | 1.00 | 39.06 | 6 |
| | ATOM | 5582 | CG | TRP | D | 82 | 56.206 | 60.891 | 13.958 | 1.00 | 40.02 | 6 |
| | ATOM | 5583 | CD2 | TRP | D | 82 | 56.715 | 61.864 | 14.887 | 1.00 | 39.10 | 6 |
| | ATOM | 5584 | CE2 | TRP | D | 82 | 57.878 | 61.318 | 15.463 | 1.00 | 38.66 | 6 |
| 45 | ATOM | 5585 | CE3 | TRP | D | 82 | 56.294 | 63.140 | 15.292 | 1.00 | 38.90 | 6 |
| | ATOM | 5586 | CD1 | TRP | D | 82 | 57.060 | 59.840 | 14.007 | 1.00 | 40.23 | 6 |
| | ATOM | 5587 | NE1 | TRP | D | 82 | 58.065 | 60.082 | 14.908 | 1.00 | 40.21 | 7 |
| | ATOM | 5588 | CZ2 | TRP | D | 82 | 58.630 | 61.997 | 16.422 | 1.00 | 36.80 | 6 |
| | ATOM | 5589 | CZ3 | TRP | D | 82 | 57.038 | 63.812 | 16.247 | 1.00 | 40.18 | 6 |
| 50 | ATOM | 5590 | CH2 | TRP | D | 82 | 58.195 | 63.238 | 16.801 | 1.00 | 38.54 | 6 |
| | ATOM | 5591 | C | TRP | D | 82 | 53.606 | 61.068 | 15.236 | 1.00 | 35.47 | 6 |
| | ATOM | 5592 | O | TRP | D | 82 | 53.085 | 62.172 | 15.339 | 1.00 | 36.72 | 8 |
| | ATOM | 5593 | N | VAL | D | 83 | 54.078 | 60.408 | 16.272 | 1.00 | 34.62 | 7 |
| | ATOM | 5594 | CA | VAL | D | 83 | 53.996 | 60.989 | 17.592 | 1.00 | 36.17 | 6 |
| 55 | ATOM | 5595 | CB | VAL | D | 83 | 52.827 | 60.341 | 18.381 | 1.00 | 35.89 | 6 |
| | ATOM | 5596 | CG1 | VAL | D | 83 | 52.906 | 60.676 | 19.835 | 1.00 | 38.30 | 6 |
| | ATOM | 5597 | CG2 | VAL | D | 83 | 51.507 | 60.840 | 17.832 | 1.00 | 35.92 | 6 |
| | ATOM | 5598 | C | VAL | D | 83 | 55.335 | 60.810 | 18.312 | 1.00 | 37.27 | 6 |
| | ATOM | 5599 | O | VAL | D | 83 | 56.035 | 59.821 | 18.113 | 1.00 | 36.95 | 8 |
| 60 | ATOM | 5600 | N | PRO | D | 84 | 55.727 | 61.796 | 19.125 | 1.00 | 35.49 | 7 |
| | ATOM | 5601 | CD | PRO | D | 84 | 55.073 | 63.095 | 19.324 | 1.00 | 37.20 | 6 |

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|----|------|------|-----|-----|------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 5602 | CA | PRO | D 84 | 56.979 | 61.740 | 19.873 | 1.00 | 36.59 | 6 |
| | ATOM | 5603 | CB | PRO | D 84 | 56.933 | 63.024 | 20.694 | 1.00 | 37.18 | 6 |
| | ATOM | 5604 | CG | PRO | D 84 | 56.196 | 63.930 | 19.835 | 1.00 | 36.05 | 6 |
| | ATOM | 5605 | C | PRO | D 84 | 57.034 | 60.502 | 20.759 | 1.00 | 35.92 | 6 |
| | ATOM | 5606 | O | PRO | D 84 | 56.070 | 60.197 | 21.449 | 1.00 | 34.78 | 8 |
| 10 | ATOM | 5607 | N | ASP | D 85 | 58.161 | 59.798 | 20.749 | 1.00 | 33.98 | 7 |
| | ATOM | 5608 | CA | ASP | D 85 | 58.283 | 58.609 | 21.565 | 1.00 | 34.25 | 6 |
| | ATOM | 5609 | CB | ASP | D 85 | 59.244 | 57.622 | 20.925 | 1.00 | 35.35 | 6 |
| | ATOM | 5610 | CG | ASP | D 85 | 60.600 | 58.201 | 20.700 | 1.00 | 38.15 | 6 |
| | ATOM | 5611 | OD1 | ASP | D 85 | 60.645 | 59.379 | 20.327 | 1.00 | 40.37 | 8 |
| 15 | ATOM | 5612 | OD2 | ASP | D 85 | 61.612 | 57.486 | 20.870 | 1.00 | 36.29 | 8 |
| | ATOM | 5613 | C | ASP | D 85 | 58.740 | 58.962 | 22.964 | 1.00 | 37.26 | 6 |
| | ATOM | 5614 | O | ASP | D 85 | 59.737 | 58.449 | 23.453 | 1.00 | 38.45 | 8 |
| | ATOM | 5615 | N | LEU | D 86 | 57.981 | 59.840 | 23.609 | 1.00 | 35.72 | 7 |
| | ATOM | 5616 | CA | LEU | D 86 | 58.290 | 60.294 | 24.956 | 1.00 | 37.34 | 6 |
| 20 | ATOM | 5617 | CB | LEU | D 86 | 57.397 | 61.471 | 25.325 | 1.00 | 35.58 | 6 |
| | ATOM | 5618 | CG | LEU | D 86 | 57.576 | 62.690 | 24.434 | 1.00 | 36.77 | 6 |
| | ATOM | 5619 | CD1 | LEU | D 86 | 56.652 | 63.799 | 24.877 | 1.00 | 32.58 | 6 |
| | ATOM | 5620 | CD2 | LEU | D 86 | 59.026 | 63.127 | 24.496 | 1.00 | 36.92 | 6 |
| | ATOM | 5621 | C | LEU | D 86 | 58.112 | 59.205 | 25.989 | 1.00 | 38.80 | 6 |
| 25 | ATOM | 5622 | O | LEU | D 86 | 57.250 | 58.337 | 25.853 | 1.00 | 43.05 | 8 |
| | ATOM | 5623 | N | ALA | D 87 | 58.925 | 59.263 | 27.033 | 1.00 | 38.29 | 7 |
| | ATOM | 5624 | CA | ALA | D 87 | 58.852 | 58.291 | 28.103 | 1.00 | 38.34 | 6 |
| | ATOM | 5625 | CB | ALA | D 87 | 59.808 | 57.174 | 27.827 | 1.00 | 37.03 | 6 |
| | ATOM | 5626 | C | ALA | D 87 | 59.202 | 58.966 | 29.414 | 1.00 | 39.60 | 6 |
| 30 | ATOM | 5627 | O | ALA | D 87 | 60.087 | 59.793 | 29.436 | 1.00 | 43.32 | 8 |
| | ATOM | 5628 | N | ALA | D 88 | 58.495 | 58.644 | 30.492 | 1.00 | 39.86 | 7 |
| | ATOM | 5629 | CA | ALA | D 88 | 58.804 | 59.234 | 31.786 | 1.00 | 39.70 | 6 |
| | ATOM | 5630 | CB | ALA | D 88 | 57.572 | 59.294 | 32.654 | 1.00 | 38.81 | 6 |
| | ATOM | 5631 | C | ALA | D 88 | 59.861 | 58.347 | 32.418 | 1.00 | 41.02 | 6 |
| 35 | ATOM | 5632 | O | ALA | D 88 | 59.575 | 57.259 | 32.894 | 1.00 | 42.74 | 8 |
| | ATOM | 5633 | N | TYR | D 89 | 61.095 | 58.826 | 32.400 | 1.00 | 42.88 | 7 |
| | ATOM | 5634 | CA | TYR | D 89 | 62.241 | 58.101 | 32.931 | 1.00 | 44.50 | 6 |
| | ATOM | 5635 | CB | TYR | D 89 | 63.443 | 59.050 | 33.031 | 1.00 | 46.85 | 6 |
| | ATOM | 5636 | CG | TYR | D 89 | 63.940 | 59.583 | 31.709 | 1.00 | 50.97 | 6 |
| 40 | ATOM | 5637 | CD1 | TYR | D 89 | 64.910 | 60.571 | 31.663 | 1.00 | 55.21 | 6 |
| | ATOM | 5638 | CE1 | TYR | D 89 | 65.384 | 61.063 | 30.441 | 1.00 | 57.34 | 6 |
| | ATOM | 5639 | CD2 | TYR | D 89 | 63.452 | 59.090 | 30.502 | 1.00 | 52.68 | 6 |
| | ATOM | 5640 | CE2 | TYR | D 89 | 63.916 | 59.569 | 29.288 | 1.00 | 55.92 | 6 |
| | ATOM | 5641 | CZ | TYR | D 89 | 64.881 | 60.557 | 29.260 | 1.00 | 57.40 | 6 |
| 45 | ATOM | 5642 | OH | TYR | D 89 | 65.341 | 61.041 | 28.048 | 1.00 | 61.62 | 8 |
| | ATOM | 5643 | C | TYR | D 89 | 62.044 | 57.403 | 34.274 | 1.00 | 43.55 | 6 |
| | ATOM | 5644 | O | TYR | D 89 | 62.618 | 56.340 | 34.503 | 1.00 | 43.31 | 8 |
| | ATOM | 5645 | N | ASN | D 90 | 61.261 | 57.992 | 35.171 | 1.00 | 40.99 | 7 |
| | ATOM | 5646 | CA | ASN | D 90 | 61.059 | 57.368 | 36.470 | 1.00 | 40.89 | 6 |
| 50 | ATOM | 5647 | CB | ASN | D 90 | 61.459 | 58.323 | 37.605 | 1.00 | 38.07 | 6 |
| | ATOM | 5648 | CG | ASN | D 90 | 60.717 | 59.639 | 37.561 | 1.00 | 38.20 | 6 |
| | ATOM | 5649 | OD1 | ASN | D 90 | 60.602 | 60.270 | 36.515 | 1.00 | 43.00 | 8 |
| | ATOM | 5650 | ND2 | ASN | D 90 | 60.229 | 60.071 | 38.707 | 1.00 | 36.31 | 7 |
| | ATOM | 5651 | C | ASN | D 90 | 59.646 | 56.851 | 36.669 | 1.00 | 41.76 | 6 |
| 55 | ATOM | 5652 | O | ASN | D 90 | 59.170 | 56.706 | 37.795 | 1.00 | 42.39 | 8 |
| | ATOM | 5653 | N | ALA | D 91 | 58.974 | 56.568 | 35.562 | 1.00 | 42.04 | 7 |
| | ATOM | 5654 | CA | ALA | D 91 | 57.631 | 56.023 | 35.630 | 1.00 | 42.57 | 6 |
| | ATOM | 5655 | CB | ALA | D 91 | 56.985 | 56.010 | 34.260 | 1.00 | 42.26 | 6 |
| | ATOM | 5656 | C | ALA | D 91 | 57.820 | 54.603 | 36.150 | 1.00 | 42.84 | 6 |
| 60 | ATOM | 5657 | O | ALA | D 91 | 58.716 | 53.882 | 35.717 | 1.00 | 41.70 | 8 |
| | ATOM | 5658 | N | ILE | D 92 | 56.963 | 54.222 | 37.084 | 1.00 | 44.08 | 7 |
| | ATOM | 5659 | CA | ILE | D 92 | 57.012 | 52.930 | 37.733 | 1.00 | 44.15 | 6 |
| | ATOM | 5660 | CB | ILE | D 92 | 56.838 | 53.166 | 39.239 | 1.00 | 48.04 | 6 |
| | ATOM | 5661 | CG2 | ILE | D 92 | 55.423 | 52.860 | 39.672 | 1.00 | 49.55 | 6 |
| | ATOM | 5662 | CG1 | ILE | D 92 | 57.827 | 52.337 | 40.032 | 1.00 | 51.37 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|--|--|--|--|
| 5 | ATOM | 5663 | CD1 | ILE D 92 | 57.559 | 52.447 | 41.544 | 1.00 | 57.95 | 6 | | | | |
| | ATOM | 5664 | C | ILE D 92 | 55.921 | 51.998 | 37.180 | 1.00 | 43.63 | 6 | | | | |
| | ATOM | 5665 | O | ILE D 92 | 55.867 | 50.816 | 37.502 | 1.00 | 43.77 | 8 | | | | |
| | ATOM | 5666 | N | SER D 93 | 55.051 | 52.546 | 36.343 | 1.00 | 41.02 | 7 | | | | |
| | ATOM | 5667 | CA | SER D 93 | 53.968 | 51.788 | 35.733 | 1.00 | 39.43 | 6 | | | | |
| 10 | ATOM | 5668 | CB | SER D 93 | 52.673 | 51.994 | 36.498 | 1.00 | 40.39 | 6 | | | | |
| | ATOM | 5669 | OG | SER D 93 | 52.200 | 53.324 | 36.320 | 1.00 | 40.98 | 8 | | | | |
| | ATOM | 5670 | C | SER D 93 | 53.802 | 52.387 | 34.366 | 1.00 | 39.82 | 6 | | | | |
| | ATOM | 5671 | O | SER D 93 | 54.349 | 53.452 | 34.103 | 1.00 | 38.78 | 8 | | | | |
| | ATOM | 5672 | N | LYS D 94 | 53.063 | 51.727 | 33.484 | 1.00 | 40.02 | 7 | | | | |
| 15 | ATOM | 5673 | CA | LYS D 94 | 52.883 | 52.322 | 32.173 | 1.00 | 42.68 | 6 | | | | |
| | ATOM | 5674 | CB | LYS D 94 | 52.695 | 51.260 | 31.081 | 1.00 | 42.12 | 6 | | | | |
| | ATOM | 5675 | CG | LYS D 94 | 51.789 | 50.113 | 31.405 | 1.00 | 45.31 | 6 | | | | |
| | ATOM | 5676 | CD | LYS D 94 | 51.980 | 48.999 | 30.378 | 1.00 | 48.12 | 6 | | | | |
| | ATOM | 5677 | CE | LYS D 94 | 51.973 | 49.545 | 28.957 | 1.00 | 49.66 | 6 | | | | |
| 20 | ATOM | 5678 | NZ | LYS D 94 | 52.092 | 48.466 | 27.938 | 1.00 | 53.06 | 7 | | | | |
| | ATOM | 5679 | C | LYS D 94 | 51.738 | 53.319 | 32.205 | 1.00 | 42.30 | 6 | | | | |
| | ATOM | 5680 | O | LYS D 94 | 50.899 | 53.299 | 33.104 | 1.00 | 42.15 | 8 | | | | |
| | ATOM | 5681 | N | PRO D 95 | 51.707 | 54.230 | 31.234 | 1.00 | 41.20 | 7 | | | | |
| | ATOM | 5682 | CD | PRO D 95 | 52.637 | 54.379 | 30.108 | 1.00 | 37.85 | 6 | | | | |
| 25 | ATOM | 5683 | CA | PRO D 95 | 50.655 | 55.243 | 31.178 | 1.00 | 40.86 | 6 | | | | |
| | ATOM | 5684 | CB | PRO D 95 | 51.064 | 56.117 | 29.990 | 1.00 | 41.55 | 6 | | | | |
| | ATOM | 5685 | CG | PRO D 95 | 52.512 | 55.834 | 29.821 | 1.00 | 42.69 | 6 | | | | |
| | ATOM | 5686 | C | PRO D 95 | 49.263 | 54.691 | 30.981 | 1.00 | 39.96 | 6 | | | | |
| | ATOM | 5687 | O | PRO D 95 | 49.030 | 53.893 | 30.080 | 1.00 | 39.70 | 8 | | | | |
| 30 | ATOM | 5688 | N | GLU D 96 | 48.344 | 55.113 | 31.835 | 1.00 | 40.14 | 7 | | | | |
| | ATOM | 5689 | CA | GLU D 96 | 46.961 | 54.718 | 31.689 | 1.00 | 38.41 | 6 | | | | |
| | ATOM | 5690 | CB | GLU D 96 | 46.321 | 54.399 | 33.041 | 1.00 | 40.63 | 6 | | | | |
| | ATOM | 5691 | CG | GLU D 96 | 44.880 | 53.856 | 32.923 | 1.00 | 48.74 | 6 | | | | |
| | ATOM | 5692 | CD | GLU D 96 | 44.232 | 53.503 | 34.273 | 1.00 | 51.27 | 6 | | | | |
| 35 | ATOM | 5693 | OE1 | GLU D 96 | 44.983 | 53.350 | 35.261 | 1.00 | 50.19 | 8 | | | | |
| | ATOM | 5694 | OE2 | GLU D 96 | 42.979 | 53.360 | 34.345 | 1.00 | 50.07 | 8 | | | | |
| | ATOM | 5695 | C | GLU D 96 | 46.324 | 55.963 | 31.084 | 1.00 | 37.34 | 6 | | | | |
| | ATOM | 5696 | O | GLU D 96 | 45.998 | 56.900 | 31.799 | 1.00 | 36.63 | 8 | | | | |
| | ATOM | 5697 | N | VAL D 97 | 46.199 | 55.988 | 29.760 | 1.00 | 34.71 | 7 | | | | |
| 40 | ATOM | 5698 | CA | VAL D 97 | 45.599 | 57.120 | 29.079 | 1.00 | 32.69 | 6 | | | | |
| | ATOM | 5699 | CB | VAL D 97 | 45.881 | 57.066 | 27.582 | 1.00 | 30.58 | 6 | | | | |
| | ATOM | 5700 | CG1 | VAL D 97 | 45.289 | 58.260 | 26.896 | 1.00 | 30.36 | 6 | | | | |
| | ATOM | 5701 | CG2 | VAL D 97 | 47.361 | 57.037 | 27.354 | 1.00 | 28.89 | 6 | | | | |
| | ATOM | 5702 | C | VAL D 97 | 44.104 | 57.067 | 29.345 | 1.00 | 34.47 | 6 | | | | |
| 45 | ATOM | 5703 | O | VAL D 97 | 43.431 | 56.124 | 28.962 | 1.00 | 35.88 | 8 | | | | |
| | ATOM | 5704 | N | LEU D 98 | 43.597 | 58.091 | 30.019 | 1.00 | 35.68 | 7 | | | | |
| | ATOM | 5705 | CA | LEU D 98 | 42.190 | 58.174 | 30.401 | 1.00 | 36.36 | 6 | | | | |
| | ATOM | 5706 | CB | LEU D 98 | 42.071 | 58.943 | 31.713 | 1.00 | 35.92 | 6 | | | | |
| | ATOM | 5707 | CG | LEU D 98 | 42.941 | 58.547 | 32.894 | 1.00 | 36.85 | 6 | | | | |
| 50 | ATOM | 5708 | CD1 | LEU D 98 | 42.906 | 59.639 | 33.914 | 1.00 | 35.58 | 6 | | | | |
| | ATOM | 5709 | CD2 | LEU D 98 | 42.456 | 57.261 | 33.487 | 1.00 | 39.84 | 6 | | | | |
| | ATOM | 5710 | C | LEU D 98 | 41.276 | 58.845 | 29.386 | 1.00 | 38.24 | 6 | | | | |
| | ATOM | 5711 | O | LEU D 98 | 40.055 | 58.850 | 29.549 | 1.00 | 37.04 | 8 | | | | |
| | ATOM | 5712 | N | THR D 99 | 41.862 | 59.409 | 28.338 | 1.00 | 37.00 | 7 | | | | |
| 55 | ATOM | 5713 | CA | THR D 99 | 41.082 | 60.130 | 27.344 | 1.00 | 36.28 | 6 | | | | |
| | ATOM | 5714 | CB | THR D 99 | 41.449 | 61.644 | 27.378 | 1.00 | 36.19 | 6 | | | | |
| | ATOM | 5715 | OG1 | THR D 99 | 42.863 | 61.803 | 27.177 | 1.00 | 38.29 | 8 | | | | |
| | ATOM | 5716 | CG2 | THR D 99 | 41.075 | 62.248 | 28.706 | 1.00 | 31.31 | 6 | | | | |
| | ATOM | 5717 | C | THR D 99 | 41.224 | 59.629 | 25.910 | 1.00 | 35.89 | 6 | | | | |
| 60 | ATOM | 5718 | O | THR D 99 | 42.148 | 58.883 | 25.588 | 1.00 | 35.45 | 8 | | | | |
| | ATOM | 5719 | N | PRO D 100 | 40.281 | 60.026 | 25.034 | 1.00 | 34.88 | 7 | | | | |
| | ATOM | 5720 | CD | PRO D 100 | 39.043 | 60.761 | 25.337 | 1.00 | 35.25 | 6 | | | | |
| | ATOM | 5721 | CA | PRO D 100 | 40.303 | 59.630 | 23.631 | 1.00 | 33.36 | 6 | | | | |
| | ATOM | 5722 | CB | PRO D 100 | 39.217 | 60.492 | 23.024 | 1.00 | 32.41 | 6 | | | | |
| | ATOM | 5723 | CG | PRO D 100 | 38.223 | 60.527 | 24.093 | 1.00 | 33.73 | 6 | | | | |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 5724 | C PRO D 100 | 41.666 | 59.955 | 23.077 | 1.00 | 35.04 | 6 | |
| | ATOM | 5725 | O PRO D 100 | 42.188 | 61.028 | 23.310 | 1.00 | 36.02 | 8 | |
| | ATOM | 5726 | N GLN D 101 | 42.256 | 59.026 | 22.350 | 1.00 | 38.56 | 7 | |
| | ATOM | 5727 | CA GLN D 101 | 43.574 | 59.280 | 21.817 | 1.00 | 39.66 | 6 | |
| | ATOM | 5728 | CB GLN D 101 | 44.356 | 57.980 | 21.749 | 1.00 | 38.98 | 6 | |
| 10 | ATOM | 5729 | CG GLN D 101 | 44.890 | 57.613 | 23.109 | 1.00 | 41.80 | 6 | |
| | ATOM | 5730 | CD GLN D 101 | 45.318 | 56.175 | 23.201 | 1.00 | 46.38 | 6 | |
| | ATOM | 5731 | OE1 GLN D 101 | 46.158 | 55.714 | 22.439 | 1.00 | 50.42 | 8 | |
| | ATOM | 5732 | NE2 GLN D 101 | 44.735 | 55.447 | 24.143 | 1.00 | 49.13 | 7 | |
| | ATOM | 5733 | C GLN D 101 | 43.543 | 59.994 | 20.486 | 1.00 | 39.27 | 6 | |
| 15 | ATOM | 5734 | O GLN D 101 | 43.965 | 59.463 | 19.463 | 1.00 | 38.19 | 8 | |
| | ATOM | 5735 | N LEU D 102 | 43.037 | 61.224 | 20.540 | 1.00 | 40.46 | 7 | |
| | ATOM | 5736 | CA LEU D 102 | 42.910 | 62.103 | 19.381 | 1.00 | 40.51 | 6 | |
| | ATOM | 5737 | CB LEU D 102 | 41.467 | 62.590 | 19.231 | 1.00 | 37.39 | 6 | |
| | ATOM | 5738 | CG LEU D 102 | 40.382 | 61.515 | 19.121 | 1.00 | 38.97 | 6 | |
| 20 | ATOM | 5739 | CD1 LEU D 102 | 39.030 | 62.182 | 18.988 | 1.00 | 36.48 | 6 | |
| | ATOM | 5740 | CD2 LEU D 102 | 40.657 | 60.628 | 17.925 | 1.00 | 36.34 | 6 | |
| | ATOM | 5741 | C LEU D 102 | 43.804 | 63.308 | 19.554 | 1.00 | 41.42 | 6 | |
| | ATOM | 5742 | O LEU D 102 | 43.990 | 63.794 | 20.665 | 1.00 | 43.09 | 8 | |
| | ATOM | 5743 | N ALA D 103 | 44.375 | 63.777 | 18.455 | 1.00 | 40.44 | 7 | |
| 25 | ATOM | 5744 | CA ALA D 103 | 45.221 | 64.953 | 18.489 | 1.00 | 40.53 | 6 | |
| | ATOM | 5745 | CB ALA D 103 | 46.549 | 64.673 | 17.847 | 1.00 | 43.43 | 6 | |
| | ATOM | 5746 | C ALA D 103 | 44.500 | 66.050 | 17.731 | 1.00 | 41.82 | 6 | |
| | ATOM | 5747 | O ALA D 103 | 43.503 | 65.803 | 17.058 | 1.00 | 41.33 | 8 | |
| | ATOM | 5748 | N ARG D 104 | 44.998 | 67.271 | 17.849 | 1.00 | 42.58 | 7 | |
| 30 | ATOM | 5749 | CA ARG D 104 | 44.369 | 68.381 | 17.165 | 1.00 | 43.20 | 6 | |
| | ATOM | 5750 | CB ARG D 104 | 43.995 | 69.450 | 18.183 | 1.00 | 43.57 | 6 | |
| | ATOM | 5751 | CG ARG D 104 | 43.032 | 70.480 | 17.678 | 1.00 | 40.98 | 6 | |
| | ATOM | 5752 | CD ARG D 104 | 41.674 | 69.900 | 17.425 | 1.00 | 39.96 | 6 | |
| | ATOM | 5753 | NE ARG D 104 | 40.803 | 70.951 | 16.909 | 1.00 | 41.32 | 7 | |
| 35 | ATOM | 5754 | CZ ARG D 104 | 39.517 | 70.802 | 16.635 | 1.00 | 39.52 | 6 | |
| | ATOM | 5755 | NH1 ARG D 104 | 38.927 | 69.633 | 16.824 | 1.00 | 40.96 | 7 | |
| | ATOM | 5756 | NH2 ARG D 104 | 38.826 | 71.832 | 16.175 | 1.00 | 38.44 | 7 | |
| | ATOM | 5757 | C ARG D 104 | 45.380 | 68.896 | 16.162 | 1.00 | 43.89 | 6 | |
| | ATOM | 5758 | O ARG D 104 | 46.508 | 69.192 | 16.526 | 1.00 | 44.97 | 8 | |
| 40 | ATOM | 5759 | N VAL D 105 | 44.989 | 68.966 | 14.894 | 1.00 | 44.88 | 7 | |
| | ATOM | 5760 | CA VAL D 105 | 45.910 | 69.427 | 13.863 | 1.00 | 46.87 | 6 | |
| | ATOM | 5761 | CB VAL D 105 | 46.094 | 68.380 | 12.751 | 1.00 | 44.91 | 6 | |
| | ATOM | 5762 | CG1 VAL D 105 | 47.165 | 68.838 | 11.787 | 1.00 | 42.60 | 6 | |
| | ATOM | 5763 | CG2 VAL D 105 | 46.469 | 67.050 | 13.346 | 1.00 | 43.58 | 6 | |
| 45 | ATOM | 5764 | C VAL D 105 | 45.467 | 70.729 | 13.223 | 1.00 | 48.29 | 6 | |
| | ATOM | 5765 | O VAL D 105 | 44.335 | 70.845 | 12.731 | 1.00 | 47.85 | 8 | |
| | ATOM | 5766 | N VAL D 106 | 46.375 | 71.702 | 13.238 | 1.00 | 48.47 | 7 | |
| | ATOM | 5767 | CA VAL D 106 | 46.129 | 73.018 | 12.663 | 1.00 | 50.73 | 6 | |
| | ATOM | 5768 | CB VAL D 106 | 46.855 | 74.106 | 13.472 | 1.00 | 50.55 | 6 | |
| 50 | ATOM | 5769 | CG1 VAL D 106 | 46.392 | 75.477 | 13.026 | 1.00 | 51.23 | 6 | |
| | ATOM | 5770 | CG2 VAL D 106 | 46.601 | 73.903 | 14.951 | 1.00 | 48.01 | 6 | |
| | ATOM | 5771 | C VAL D 106 | 46.636 | 73.025 | 11.216 | 1.00 | 51.91 | 6 | |
| | ATOM | 5772 | O VAL D 106 | 47.664 | 72.420 | 10.918 | 1.00 | 52.36 | 8 | |
| | ATOM | 5773 | N SER D 107 | 45.920 | 73.712 | 10.329 | 1.00 | 52.06 | 7 | |
| 55 | ATOM | 5774 | CA SER D 107 | 46.281 | 73.761 | 8.915 | 1.00 | 51.56 | 6 | |
| | ATOM | 5775 | CB SER D 107 | 45.391 | 74.756 | 8.185 | 1.00 | 52.91 | 6 | |
| | ATOM | 5776 | OG SER D 107 | 45.259 | 75.941 | 8.943 | 1.00 | 59.44 | 8 | |
| | ATOM | 5777 | C SER D 107 | 47.726 | 74.058 | 8.591 | 1.00 | 50.83 | 6 | |
| | ATOM | 5778 | O SER D 107 | 48.188 | 73.739 | 7.511 | 1.00 | 50.82 | 8 | |
| 60 | ATOM | 5779 | N ASP D 108 | 48.451 | 74.657 | 9.519 | 1.00 | 53.72 | 7 | |
| | ATOM | 5780 | CA ASP D 108 | 49.853 | 74.978 | 9.262 | 1.00 | 57.12 | 6 | |
| | ATOM | 5781 | CB ASP D 108 | 50.239 | 76.289 | 9.965 | 1.00 | 58.24 | 6 | |
| | ATOM | 5782 | CG ASP D 108 | 50.271 | 76.163 | 11.475 | 1.00 | 61.04 | 6 | |
| | ATOM | 5783 | OD1 ASP D 108 | 49.396 | 75.459 | 12.042 | 1.00 | 63.89 | 8 | |
| | ATOM | 5784 | OD2 ASP D 108 | 51.162 | 76.782 | 12.095 | 1.00 | 60.97 | 8 | |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|----|
| 5 | ATOM | 5785 | C | ASP D 108 | 50.827 | 73.870 | 9.665 | 1.00 | 58.88 | 6 |
| | ATOM | 5786 | O | ASP D 108 | 52.043 | 74.071 | 9.635 | 1.00 | 61.62 | 8 |
| | ATOM | 5787 | N | GLY D 109 | 50.293 | 72.711 | 10.051 | 1.00 | 58.94 | 7 |
| | ATOM | 5788 | CA | GLY D 109 | 51.134 | 71.589 | 10.437 | 1.00 | 58.18 | 6 |
| | ATOM | 5789 | C | GLY D 109 | 51.424 | 71.483 | 11.918 | 1.00 | 57.62 | 6 |
| 10 | ATOM | 5790 | O | GLY D 109 | 52.186 | 70.612 | 12.343 | 1.00 | 56.21 | 8 |
| | ATOM | 5791 | N | GLU D 110 | 50.831 | 72.370 | 12.707 | 1.00 | 58.61 | 7 |
| | ATOM | 5792 | CA | GLU D 110 | 51.042 | 72.345 | 14.152 | 1.00 | 59.21 | 6 |
| | ATOM | 5793 | CB | GLU D 110 | 50.664 | 73.700 | 14.776 | 1.00 | 62.41 | 6 |
| | ATOM | 5794 | CG | GLU D 110 | 51.327 | 74.002 | 16.134 | 1.00 | 66.58 | 6 |
| 15 | ATOM | 5795 | CD | GLU D 110 | 52.852 | 74.104 | 16.041 | 1.00 | 69.79 | 6 |
| | ATOM | 5796 | OE1 | GLU D 110 | 53.375 | 74.340 | 14.921 | 1.00 | 70.58 | 8 |
| | ATOM | 5797 | OE2 | GLU D 110 | 53.527 | 73.963 | 17.089 | 1.00 | 70.10 | 8 |
| | ATOM | 5798 | C | GLU D 110 | 50.158 | 71.232 | 14.712 | 1.00 | 56.76 | 6 |
| | ATOM | 5799 | O | GLU D 110 | 49.001 | 71.079 | 14.320 | 1.00 | 54.86 | 8 |
| 20 | ATOM | 5800 | N | VAL D 111 | 50.723 | 70.451 | 15.625 | 1.00 | 55.23 | 7 |
| | ATOM | 5801 | CA | VAL D 111 | 50.013 | 69.333 | 16.236 | 1.00 | 53.43 | 6 |
| | ATOM | 5802 | CB | VAL D 111 | 50.704 | 67.976 | 15.889 | 1.00 | 53.47 | 6 |
| | ATOM | 5803 | CG1 | VAL D 111 | 49.934 | 66.821 | 16.500 | 1.00 | 51.83 | 6 |
| | ATOM | 5804 | CG2 | VAL D 111 | 50.798 | 67.803 | 14.382 | 1.00 | 52.57 | 6 |
| 25 | ATOM | 5805 | C | VAL D 111 | 49.962 | 69.470 | 17.754 | 1.00 | 53.05 | 6 |
| | ATOM | 5806 | O | VAL D 111 | 50.972 | 69.747 | 18.400 | 1.00 | 52.81 | 8 |
| | ATOM | 5807 | N | LEU D 112 | 48.783 | 69.269 | 18.323 | 1.00 | 51.91 | 7 |
| | ATOM | 5808 | CA | LEU D 112 | 48.631 | 69.354 | 19.766 | 1.00 | 51.71 | 6 |
| | ATOM | 5809 | CB | LEU D 112 | 47.776 | 70.566 | 20.155 | 1.00 | 55.12 | 6 |
| 30 | ATOM | 5810 | CG | LEU D 112 | 47.832 | 71.901 | 19.392 | 1.00 | 55.82 | 6 |
| | ATOM | 5811 | CD1 | LEU D 112 | 49.269 | 72.287 | 19.035 | 1.00 | 56.65 | 6 |
| | ATOM | 5812 | CD2 | LEU D 112 | 46.985 | 71.777 | 18.155 | 1.00 | 55.54 | 6 |
| | ATOM | 5813 | C | LEU D 112 | 47.959 | 68.089 | 20.292 | 1.00 | 51.46 | 6 |
| | ATOM | 5814 | O | LEU D 112 | 46.833 | 67.769 | 19.900 | 1.00 | 51.33 | 8 |
| 35 | ATOM | 5815 | N | TYR D 113 | 48.659 | 67.365 | 21.162 | 1.00 | 48.43 | 7 |
| | ATOM | 5816 | CA | TYR D 113 | 48.128 | 66.149 | 21.762 | 1.00 | 45.71 | 6 |
| | ATOM | 5817 | CB | TYR D 113 | 48.941 | 64.928 | 21.318 | 1.00 | 43.52 | 6 |
| | ATOM | 5818 | CG | TYR D 113 | 48.490 | 63.601 | 21.918 | 1.00 | 41.37 | 6 |
| | ATOM | 5819 | CD1 | TYR D 113 | 47.142 | 63.255 | 21.975 | 1.00 | 39.60 | 6 |
| 40 | ATOM | 5820 | CE1 | TYR D 113 | 46.735 | 62.028 | 22.492 | 1.00 | 38.43 | 6 |
| | ATOM | 5821 | CD2 | TYR D 113 | 49.423 | 62.679 | 22.397 | 1.00 | 40.11 | 6 |
| | ATOM | 5822 | CE2 | TYR D 113 | 49.028 | 61.458 | 22.911 | 1.00 | 39.17 | 6 |
| | ATOM | 5823 | CZ | TYR D 113 | 47.682 | 61.134 | 22.958 | 1.00 | 40.31 | 6 |
| | ATOM | 5824 | OH | TYR D 113 | 47.283 | 59.921 | 23.470 | 1.00 | 40.08 | 8 |
| 45 | ATOM | 5825 | C | TYR D 113 | 48.218 | 66.325 | 23.262 | 1.00 | 45.22 | 6 |
| | ATOM | 5826 | O | TYR D 113 | 49.302 | 66.442 | 23.812 | 1.00 | 44.34 | 8 |
| | ATOM | 5827 | N | MET D 114 | 47.073 | 66.352 | 23.924 | 1.00 | 47.16 | 7 |
| | ATOM | 5828 | CA | MET D 114 | 47.044 | 66.541 | 25.368 | 1.00 | 48.56 | 6 |
| | ATOM | 5829 | CB | MET D 114 | 46.457 | 67.906 | 25.681 | 1.00 | 53.17 | 6 |
| 50 | ATOM | 5830 | CG | MET D 114 | 46.536 | 68.281 | 27.130 | 1.00 | 58.47 | 6 |
| | ATOM | 5831 | SD | MET D 114 | 45.470 | 69.687 | 27.429 | 1.00 | 64.86 | 16 |
| | ATOM | 5832 | CE | MET D 114 | 46.527 | 70.991 | 26.840 | 1.00 | 63.87 | 6 |
| | ATOM | 5833 | C | MET D 114 | 46.214 | 65.472 | 26.062 | 1.00 | 47.72 | 6 |
| | ATOM | 5834 | O | MET D 114 | 45.060 | 65.705 | 26.424 | 1.00 | 47.31 | 8 |
| 55 | ATOM | 5835 | N | PRO D 115 | 46.790 | 64.279 | 26.251 | 1.00 | 45.85 | 7 |
| | ATOM | 5836 | CD | PRO D 115 | 48.108 | 63.831 | 25.761 | 1.00 | 45.44 | 6 |
| | ATOM | 5837 | CA | PRO D 115 | 46.080 | 63.184 | 26.903 | 1.00 | 44.65 | 6 |
| | ATOM | 5838 | CB | PRO D 115 | 46.818 | 61.967 | 26.385 | 1.00 | 46.29 | 6 |
| | ATOM | 5839 | CG | PRO D 115 | 48.231 | 62.454 | 26.372 | 1.00 | 45.12 | 6 |
| 60 | ATOM | 5840 | C | PRO D 115 | 46.159 | 63.283 | 28.416 | 1.00 | 44.40 | 6 |
| | ATOM | 5841 | O | PRO D 115 | 47.145 | 63.787 | 28.954 | 1.00 | 43.35 | 8 |
| | ATOM | 5842 | N | SER D 116 | 45.124 | 62.811 | 29.102 | 1.00 | 42.71 | 7 |
| | ATOM | 5843 | CA | SER D 116 | 45.142 | 62.828 | 30.551 | 1.00 | 40.50 | 6 |
| | ATOM | 5844 | CB | SER D 116 | 43.752 | 62.976 | 31.110 | 1.00 | 37.94 | 6 |
| | ATOM | 5845 | OG | SER D 116 | 43.829 | 63.015 | 32.516 | 1.00 | 44.37 | 8 |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 5846 | C | SER D 116 | 45.712 | 61.484 | 30.957 | 1.00 | 42.16 | 6 |
| | ATOM | 5847 | O | SER D 116 | 45.190 | 60.448 | 30.569 | 1.00 | 45.67 | 8 |
| | ATOM | 5848 | N | ILE D 117 | 46.781 | 61.493 | 31.739 | 1.00 | 39.79 | 7 |
| | ATOM | 5849 | CA | ILE D 117 | 47.409 | 60.252 | 32.135 | 1.00 | 38.51 | 6 |
| | ATOM | 5850 | CB | ILE D 117 | 48.842 | 60.179 | 31.565 | 1.00 | 38.14 | 6 |
| 10 | ATOM | 5851 | CG2 | ILE D 117 | 49.545 | 58.932 | 32.041 | 1.00 | 38.72 | 6 |
| | ATOM | 5852 | CG1 | ILE D 117 | 48.802 | 60.188 | 30.045 | 1.00 | 37.23 | 6 |
| | ATOM | 5853 | CD1 | ILE D 117 | 50.137 | 60.454 | 29.422 | 1.00 | 31.06 | 6 |
| | ATOM | 5854 | C | ILE D 117 | 47.506 | 60.000 | 33.635 | 1.00 | 40.56 | 6 |
| | ATOM | 5855 | O | ILE D 117 | 47.838 | 60.894 | 34.407 | 1.00 | 41.12 | 8 |
| 15 | ATOM | 5856 | N | ARG D 118 | 47.196 | 58.773 | 34.042 | 1.00 | 40.57 | 7 |
| | ATOM | 5857 | CA | ARG D 118 | 47.356 | 58.386 | 35.429 | 1.00 | 39.48 | 6 |
| | ATOM | 5858 | CB | ARG D 118 | 46.151 | 57.623 | 35.966 | 1.00 | 37.31 | 6 |
| | ATOM | 5859 | CG | ARG D 118 | 46.420 | 57.119 | 37.377 | 1.00 | 36.74 | 6 |
| | ATOM | 5860 | CD | ARG D 118 | 45.196 | 56.638 | 38.101 | 1.00 | 36.75 | 6 |
| 20 | ATOM | 5861 | NE | ARG D 118 | 45.554 | 56.131 | 39.414 | 1.00 | 36.89 | 7 |
| | ATOM | 5862 | CZ | ARG D 118 | 44.687 | 55.838 | 40.367 | 1.00 | 36.15 | 6 |
| | ATOM | 5863 | NH1 | ARG D 118 | 43.396 | 56.001 | 40.163 | 1.00 | 38.10 | 7 |
| | ATOM | 5864 | NH2 | ARG D 118 | 45.118 | 55.381 | 41.523 | 1.00 | 35.81 | 7 |
| | ATOM | 5865 | C | ARG D 118 | 48.581 | 57.469 | 35.376 | 1.00 | 39.50 | 6 |
| 25 | ATOM | 5866 | O | ARG D 118 | 48.661 | 56.579 | 34.541 | 1.00 | 39.41 | 8 |
| | ATOM | 5867 | N | GLN D 119 | 49.541 | 57.678 | 36.260 | 1.00 | 39.25 | 7 |
| | ATOM | 5868 | CA | GLN D 119 | 50.739 | 56.865 | 36.222 | 1.00 | 40.77 | 6 |
| | ATOM | 5869 | CB | GLN D 119 | 51.588 | 57.357 | 35.059 | 1.00 | 39.61 | 6 |
| | ATOM | 5870 | CG | GLN D 119 | 52.879 | 56.638 | 34.807 | 1.00 | 39.00 | 6 |
| 30 | ATOM | 5871 | CD | GLN D 119 | 53.483 | 57.037 | 33.476 | 1.00 | 37.41 | 6 |
| | ATOM | 5872 | OE1 | GLN D 119 | 53.349 | 58.169 | 33.043 | 1.00 | 42.14 | 8 |
| | ATOM | 5873 | NE2 | GLN D 119 | 54.154 | 56.112 | 32.831 | 1.00 | 38.80 | 7 |
| | ATOM | 5874 | C | GLN D 119 | 51.491 | 56.961 | 37.534 | 1.00 | 42.32 | 6 |
| | ATOM | 5875 | O | GLN D 119 | 51.421 | 57.965 | 38.213 | 1.00 | 43.53 | 8 |
| 35 | ATOM | 5876 | N | ARG D 120 | 52.197 | 55.908 | 37.906 | 1.00 | 43.85 | 7 |
| | ATOM | 5877 | CA | ARG D 120 | 52.950 | 55.944 | 39.149 | 1.00 | 47.43 | 6 |
| | ATOM | 5878 | CB | ARG D 120 | 52.819 | 54.632 | 39.900 | 1.00 | 50.39 | 6 |
| | ATOM | 5879 | CG | ARG D 120 | 51.389 | 54.278 | 40.235 | 1.00 | 58.64 | 6 |
| | ATOM | 5880 | CD | ARG D 120 | 51.352 | 53.441 | 41.493 | 1.00 | 64.21 | 6 |
| 40 | ATOM | 5881 | NE | ARG D 120 | 51.387 | 54.244 | 42.725 | 1.00 | 67.25 | 7 |
| | ATOM | 5882 | CZ | ARG D 120 | 52.129 | 53.942 | 43.790 | 1.00 | 65.70 | 6 |
| | ATOM | 5883 | NH1 | ARG D 120 | 52.911 | 52.870 | 43.763 | 1.00 | 64.48 | 7 |
| | ATOM | 5884 | NH2 | ARG D 120 | 52.049 | 54.678 | 44.895 | 1.00 | 62.69 | 7 |
| | ATOM | 5885 | C | ARG D 120 | 54.411 | 56.231 | 38.913 | 1.00 | 46.83 | 6 |
| 45 | ATOM | 5886 | O | ARG D 120 | 54.969 | 55.848 | 37.885 | 1.00 | 46.53 | 8 |
| | ATOM | 5887 | N | PHE D 121 | 55.032 | 56.912 | 39.869 | 1.00 | 45.77 | 7 |
| | ATOM | 5888 | CA | PHE D 121 | 56.443 | 57.249 | 39.743 | 1.00 | 45.26 | 6 |
| | ATOM | 5889 | CB | PHE D 121 | 56.627 | 58.737 | 39.416 | 1.00 | 42.47 | 6 |
| | ATOM | 5890 | CG | PHE D 121 | 55.893 | 59.186 | 38.199 | 1.00 | 41.19 | 6 |
| 50 | ATOM | 5891 | CD1 | PHE D 121 | 54.546 | 59.483 | 38.266 | 1.00 | 39.80 | 6 |
| | ATOM | 5892 | CD2 | PHE D 121 | 56.544 | 59.284 | 36.979 | 1.00 | 39.10 | 6 |
| | ATOM | 5893 | CE1 | PHE D 121 | 53.855 | 59.872 | 37.141 | 1.00 | 39.49 | 6 |
| | ATOM | 5894 | CE2 | PHE D 121 | 55.862 | 59.670 | 35.858 | 1.00 | 37.48 | 6 |
| | ATOM | 5895 | CZ | PHE D 121 | 54.512 | 59.965 | 35.937 | 1.00 | 38.89 | 6 |
| 55 | ATOM | 5896 | C | PHE D 121 | 57.256 | 56.947 | 40.980 | 1.00 | 46.08 | 6 |
| | ATOM | 5897 | O | PHE D 121 | 56.729 | 56.783 | 42.077 | 1.00 | 43.10 | 8 |
| | ATOM | 5898 | N | SER D 122 | 58.560 | 56.881 | 40.769 | 1.00 | 48.75 | 7 |
| | ATOM | 5899 | CA | SER D 122 | 59.520 | 56.672 | 41.837 | 1.00 | 51.22 | 6 |
| | ATOM | 5900 | CB | SER D 122 | 60.535 | 55.604 | 41.442 | 1.00 | 51.58 | 6 |
| 60 | ATOM | 5901 | OG | SER D 122 | 61.510 | 55.455 | 42.453 | 1.00 | 51.33 | 8 |
| | ATOM | 5902 | C | SER D 122 | 60.224 | 58.027 | 42.004 | 1.00 | 51.78 | 6 |
| | ATOM | 5903 | O | SER D 122 | 60.968 | 58.460 | 41.123 | 1.00 | 50.44 | 8 |
| | ATOM | 5904 | N | CYS D 123 | 59.965 | 58.699 | 43.120 | 1.00 | 52.36 | 7 |
| | ATOM | 5905 | CA | CYS D 123 | 60.564 | 59.999 | 43.370 | 1.00 | 55.03 | 6 |
| | ATOM | 5906 | C | CYS D 123 | 60.584 | 60.314 | 44.860 | 1.00 | 57.50 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 5907 | O | CYS | D | 123 | 60.131 | 59.513 | 45.676 | 1.00 | 58.47 | 8 |
| | ATOM | 5908 | CB | CYS | D | 123 | 59.784 | 61.083 | 42.631 | 1.00 | 54.89 | 6 |
| | ATOM | 5909 | SG | CYS | D | 123 | 58.043 | 61.147 | 43.136 | 1.00 | 52.88 | 16 |
| 5 | ATOM | 5910 | N | ASP | D | 124 | 61.104 | 61.487 | 45.218 | 1.00 | 58.85 | 7 |
| | ATOM | 5911 | CA | ASP | D | 124 | 61.196 | 61.865 | 46.619 | 1.00 | 59.59 | 6 |
| | ATOM | 5912 | CB | ASP | D | 124 | 62.205 | 62.994 | 46.816 | 1.00 | 60.38 | 6 |
| | ATOM | 5913 | CG | ASP | D | 124 | 62.876 | 62.937 | 48.182 | 1.00 | 61.57 | 6 |
| | ATOM | 5914 | OD1 | ASP | D | 124 | 62.207 | 62.519 | 49.151 | 1.00 | 60.87 | 8 |
| 10 | ATOM | 5915 | OD2 | ASP | D | 124 | 64.067 | 63.306 | 48.289 | 1.00 | 61.86 | 8 |
| | ATOM | 5916 | C | ASP | D | 124 | 59.864 | 62.294 | 47.198 | 1.00 | 59.72 | 6 |
| | ATOM | 5917 | O | ASP | D | 124 | 59.310 | 63.329 | 46.822 | 1.00 | 59.12 | 8 |
| | ATOM | 5918 | N | VAL | D | 125 | 59.366 | 61.492 | 48.131 | 1.00 | 60.02 | 7 |
| | ATOM | 5919 | CA | VAL | D | 125 | 58.096 | 61.758 | 48.795 | 1.00 | 61.00 | 6 |
| | ATOM | 5920 | CB | VAL | D | 125 | 57.274 | 60.469 | 48.906 | 1.00 | 57.98 | 6 |
| 15 | ATOM | 5921 | CG1 | VAL | D | 125 | 56.007 | 60.721 | 49.664 | 1.00 | 56.31 | 6 |
| | ATOM | 5922 | CG2 | VAL | D | 125 | 56.973 | 59.946 | 47.526 | 1.00 | 58.88 | 6 |
| | ATOM | 5923 | C | VAL | D | 125 | 58.305 | 62.346 | 50.199 | 1.00 | 63.48 | 6 |
| | ATOM | 5924 | O | VAL | D | 125 | 57.391 | 62.956 | 50.781 | 1.00 | 64.81 | 8 |
| | ATOM | 5925 | N | SER | D | 126 | 59.511 | 62.177 | 50.738 | 1.00 | 64.05 | 7 |
| 20 | ATOM | 5926 | CA | SER | D | 126 | 59.824 | 62.684 | 52.072 | 1.00 | 64.03 | 6 |
| | ATOM | 5927 | CB | SER | D | 126 | 61.317 | 62.517 | 52.362 | 1.00 | 63.15 | 6 |
| | ATOM | 5928 | OG | SER | D | 126 | 62.088 | 63.277 | 51.455 | 1.00 | 61.24 | 8 |
| | ATOM | 5929 | C | SER | D | 126 | 59.426 | 64.146 | 52.233 | 1.00 | 63.55 | 6 |
| | ATOM | 5930 | O | SER | D | 126 | 59.745 | 64.989 | 51.396 | 1.00 | 62.30 | 8 |
| 25 | ATOM | 5931 | N | GLY | D | 127 | 58.716 | 64.434 | 53.315 | 1.00 | 64.29 | 7 |
| | ATOM | 5932 | CA | GLY | D | 127 | 58.285 | 65.794 | 53.564 | 1.00 | 67.20 | 6 |
| | ATOM | 5933 | C | GLY | D | 127 | 56.868 | 66.085 | 53.115 | 1.00 | 68.64 | 6 |
| | ATOM | 5934 | O | GLY | D | 127 | 56.368 | 67.190 | 53.321 | 1.00 | 69.55 | 8 |
| | ATOM | 5935 | N | VAL | D | 128 | 56.207 | 65.103 | 52.510 | 1.00 | 70.10 | 7 |
| 30 | ATOM | 5936 | CA | VAL | D | 128 | 54.845 | 65.323 | 52.038 | 1.00 | 71.31 | 6 |
| | ATOM | 5937 | CB | VAL | D | 128 | 54.252 | 64.077 | 51.378 | 1.00 | 69.98 | 6 |
| | ATOM | 5938 | CG1 | VAL | D | 128 | 54.873 | 63.859 | 50.035 | 1.00 | 72.53 | 6 |
| | ATOM | 5939 | CG2 | VAL | D | 128 | 54.476 | 62.877 | 52.271 | 1.00 | 70.16 | 6 |
| | ATOM | 5940 | C | VAL | D | 128 | 53.883 | 65.707 | 53.136 | 1.00 | 71.70 | 6 |
| 35 | ATOM | 5941 | O | VAL | D | 128 | 53.089 | 66.634 | 52.978 | 1.00 | 69.47 | 8 |
| | ATOM | 5942 | N | ASP | D | 129 | 53.960 | 64.993 | 54.251 | 1.00 | 73.53 | 7 |
| | ATOM | 5943 | CA | ASP | D | 129 | 53.022 | 65.233 | 55.320 | 1.00 | 77.21 | 6 |
| | ATOM | 5944 | CB | ASP | D | 129 | 53.171 | 64.197 | 56.428 | 1.00 | 78.32 | 6 |
| | ATOM | 5945 | CG | ASP | D | 129 | 51.860 | 63.985 | 57.204 | 1.00 | 80.24 | 6 |
| 40 | ATOM | 5946 | OD1 | ASP | D | 129 | 51.521 | 62.805 | 57.509 | 1.00 | 81.78 | 8 |
| | ATOM | 5947 | OD2 | ASP | D | 129 | 51.172 | 64.996 | 57.504 | 1.00 | 78.07 | 8 |
| | ATOM | 5948 | C | ASP | D | 129 | 53.027 | 66.618 | 55.915 | 1.00 | 79.33 | 6 |
| | ATOM | 5949 | O | ASP | D | 129 | 52.082 | 66.963 | 56.644 | 1.00 | 80.54 | 8 |
| | ATOM | 5950 | N | THR | D | 130 | 54.041 | 67.433 | 55.604 | 1.00 | 80.13 | 7 |
| 45 | ATOM | 5951 | CA | THR | D | 130 | 54.048 | 68.779 | 56.171 | 1.00 | 80.39 | 6 |
| | ATOM | 5952 | CB | THR | D | 130 | 54.064 | 68.702 | 57.716 | 1.00 | 83.74 | 6 |
| | ATOM | 5953 | OG1 | THR | D | 130 | 54.418 | 67.359 | 58.114 | 1.00 | 84.65 | 8 |
| | ATOM | 5954 | CG2 | THR | D | 130 | 52.670 | 69.136 | 58.320 | 1.00 | 81.78 | 6 |
| | ATOM | 5955 | C | THR | D | 130 | 55.110 | 69.794 | 55.795 | 1.00 | 78.83 | 6 |
| 50 | ATOM | 5956 | O | THR | D | 130 | 56.241 | 69.440 | 55.449 | 1.00 | 77.71 | 8 |
| | ATOM | 5957 | N | GLU | D | 131 | 54.701 | 71.065 | 55.921 | 1.00 | 78.93 | 7 |
| | ATOM | 5958 | CA | GLU | D | 131 | 55.520 | 72.272 | 55.705 | 1.00 | 78.30 | 6 |
| | ATOM | 5959 | CB | GLU | D | 131 | 56.825 | 72.165 | 56.518 | 1.00 | 81.28 | 6 |
| | ATOM | 5960 | CG | GLU | D | 131 | 56.641 | 72.410 | 58.024 | 1.00 | 83.84 | 6 |
| 55 | ATOM | 5961 | CD | GLU | D | 131 | 57.696 | 71.715 | 58.856 | 1.00 | 84.29 | 6 |
| | ATOM | 5962 | OE1 | GLU | D | 131 | 58.893 | 71.821 | 58.485 | 1.00 | 85.14 | 8 |
| | ATOM | 5963 | OE2 | GLU | D | 131 | 57.321 | 71.068 | 59.870 | 1.00 | 82.70 | 8 |
| | ATOM | 5964 | C | GLU | D | 131 | 55.869 | 72.672 | 54.295 | 1.00 | 75.98 | 6 |
| | ATOM | 5965 | O | GLU | D | 131 | 55.047 | 73.205 | 53.552 | 1.00 | 74.51 | 8 |
| 60 | ATOM | 5966 | N | SER | D | 132 | 57.136 | 72.452 | 53.973 | 1.00 | 75.06 | 7 |
| | ATOM | 5967 | CA | SER | D | 132 | 57.689 | 72.733 | 52.665 | 1.00 | 74.59 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 5968 | CB | SER | D | 132 | 59.215 | 72.882 | 52.788 | 1.00 | 75.96 | 6 |
| | ATOM | 5969 | OG | SER | D | 132 | 59.812 | 71.733 | 53.401 | 1.00 | 76.36 | 8 |
| | ATOM | 5970 | C | SER | D | 132 | 57.316 | 71.551 | 51.753 | 1.00 | 72.89 | 6 |
| 5 | ATOM | 5971 | O | SER | D | 132 | 57.636 | 71.530 | 50.563 | 1.00 | 73.06 | 8 |
| | ATOM | 5972 | N | GLY | D | 133 | 56.630 | 70.575 | 52.337 | 1.00 | 70.56 | 7 |
| | ATOM | 5973 | CA | GLY | D | 133 | 56.203 | 69.406 | 51.599 | 1.00 | 67.95 | 6 |
| | ATOM | 5974 | C | GLY | D | 133 | 57.326 | 68.647 | 50.917 | 1.00 | 66.74 | 6 |
| | ATOM | 5975 | O | GLY | D | 133 | 58.504 | 68.784 | 51.257 | 1.00 | 65.57 | 8 |
| 10 | ATOM | 5976 | N | ALA | D | 134 | 56.950 | 67.830 | 49.942 | 1.00 | 65.62 | 7 |
| | ATOM | 5977 | CA | ALA | D | 134 | 57.922 | 67.052 | 49.194 | 1.00 | 63.00 | 6 |
| | ATOM | 5978 | CB | ALA | D | 134 | 57.506 | 65.586 | 49.145 | 1.00 | 62.05 | 6 |
| | ATOM | 5979 | C | ALA | D | 134 | 58.060 | 67.597 | 47.785 | 1.00 | 60.69 | 6 |
| | ATOM | 5980 | O | ALA | D | 134 | 57.215 | 68.357 | 47.298 | 1.00 | 57.71 | 8 |
| | ATOM | 5981 | N | THR | D | 135 | 59.149 | 67.206 | 47.139 | 1.00 | 60.08 | 7 |
| 15 | ATOM | 5982 | CA | THR | D | 135 | 59.417 | 67.619 | 45.777 | 1.00 | 59.14 | 6 |
| | ATOM | 5983 | CB | THR | D | 135 | 60.585 | 68.590 | 45.703 | 1.00 | 59.67 | 6 |
| | ATOM | 5984 | OG1 | THR | D | 135 | 60.291 | 69.735 | 46.516 | 1.00 | 62.19 | 8 |
| | ATOM | 5985 | CG2 | THR | D | 135 | 60.811 | 69.031 | 44.263 | 1.00 | 57.77 | 6 |
| | ATOM | 5986 | C | THR | D | 135 | 59.726 | 66.387 | 44.963 | 1.00 | 57.95 | 6 |
| 20 | ATOM | 5987 | O | THR | D | 135 | 60.801 | 65.804 | 45.065 | 1.00 | 56.51 | 8 |
| | ATOM | 5988 | N | CYS | D | 136 | 58.740 | 65.995 | 44.170 | 1.00 | 56.67 | 7 |
| | ATOM | 5989 | CA | CYS | D | 136 | 58.825 | 64.836 | 43.314 | 1.00 | 55.02 | 6 |
| | ATOM | 5990 | C | CYS | D | 136 | 59.172 | 65.310 | 41.906 | 1.00 | 55.53 | 6 |
| | ATOM | 5991 | O | CYS | D | 136 | 58.413 | 66.060 | 41.282 | 1.00 | 53.64 | 8 |
| 25 | ATOM | 5992 | CB | CYS | D | 136 | 57.475 | 64.115 | 43.347 | 1.00 | 55.35 | 6 |
| | ATOM | 5993 | SG | CYS | D | 136 | 57.280 | 62.756 | 42.175 | 1.00 | 52.04 | 16 |
| | ATOM | 5994 | N | ARG | D | 137 | 60.331 | 64.889 | 41.414 | 1.00 | 55.15 | 7 |
| | ATOM | 5995 | CA | ARG | D | 137 | 60.752 | 65.291 | 40.084 | 1.00 | 56.13 | 6 |
| | ATOM | 5996 | CB | ARG | D | 137 | 62.233 | 65.664 | 40.080 | 1.00 | 59.85 | 6 |
| 30 | ATOM | 5997 | CG | ARG | D | 137 | 62.587 | 66.818 | 40.993 | 1.00 | 64.22 | 6 |
| | ATOM | 5998 | CD | ARG | D | 137 | 64.042 | 66.718 | 41.445 | 1.00 | 67.87 | 6 |
| | ATOM | 5999 | NE | ARG | D | 137 | 64.261 | 67.425 | 42.706 | 1.00 | 72.81 | 7 |
| | ATOM | 6000 | CZ | ARG | D | 137 | 64.221 | 68.753 | 42.848 | 1.00 | 76.15 | 6 |
| | ATOM | 6001 | NH1 | ARG | D | 137 | 63.975 | 69.545 | 41.798 | 1.00 | 76.59 | 7 |
| 35 | ATOM | 6002 | NH2 | ARG | D | 137 | 64.408 | 69.295 | 44.051 | 1.00 | 75.96 | 7 |
| | ATOM | 6003 | C | ARG | D | 137 | 60.511 | 64.156 | 39.112 | 1.00 | 54.79 | 6 |
| | ATOM | 6004 | O | ARG | D | 137 | 60.844 | 63.011 | 39.394 | 1.00 | 55.64 | 8 |
| | ATOM | 6005 | N | ILE | D | 138 | 59.935 | 64.498 | 37.966 | 1.00 | 52.46 | 7 |
| | ATOM | 6006 | CA | ILE | D | 138 | 59.618 | 63.551 | 36.923 | 1.00 | 49.86 | 6 |
| 40 | ATOM | 6007 | CB | ILE | D | 138 | 58.092 | 63.516 | 36.686 | 1.00 | 47.60 | 6 |
| | ATOM | 6008 | CG2 | ILE | D | 138 | 57.769 | 62.562 | 35.565 | 1.00 | 46.55 | 6 |
| | ATOM | 6009 | CG1 | ILE | D | 138 | 57.368 | 63.120 | 37.975 | 1.00 | 44.38 | 6 |
| | ATOM | 6010 | CD1 | ILE | D | 138 | 55.873 | 63.274 | 37.903 | 1.00 | 39.29 | 6 |
| | ATOM | 6011 | C | ILE | D | 138 | 60.307 | 64.004 | 35.645 | 1.00 | 50.53 | 6 |
| 45 | ATOM | 6012 | O | ILE | D | 138 | 60.056 | 65.103 | 35.163 | 1.00 | 47.86 | 8 |
| | ATOM | 6013 | N | LYS | D | 139 | 61.171 | 63.158 | 35.093 | 1.00 | 52.17 | 7 |
| | ATOM | 6014 | CA | LYS | D | 139 | 61.881 | 63.497 | 33.857 | 1.00 | 53.46 | 6 |
| | ATOM | 6015 | CB | LYS | D | 139 | 63.381 | 63.195 | 33.988 | 1.00 | 54.96 | 6 |
| | ATOM | 6016 | CG | LYS | D | 139 | 64.040 | 63.838 | 35.187 | 1.00 | 59.06 | 6 |
| 50 | ATOM | 6017 | CD | LYS | D | 139 | 65.558 | 63.761 | 35.119 | 1.00 | 60.55 | 6 |
| | ATOM | 6018 | CE | LYS | D | 139 | 66.116 | 64.685 | 34.044 | 1.00 | 62.84 | 6 |
| | ATOM | 6019 | NZ | LYS | D | 139 | 67.604 | 64.584 | 33.930 | 1.00 | 64.96 | 7 |
| | ATOM | 6020 | C | LYS | D | 139 | 61.335 | 62.715 | 32.667 | 1.00 | 52.45 | 6 |
| | ATOM | 6021 | O | LYS | D | 139 | 61.269 | 61.493 | 32.708 | 1.00 | 52.48 | 8 |
| 55 | ATOM | 6022 | N | ILE | D | 140 | 60.953 | 63.411 | 31.604 | 1.00 | 51.17 | 7 |
| | ATOM | 6023 | CA | ILE | D | 140 | 60.453 | 62.723 | 30.426 | 1.00 | 51.40 | 6 |
| | ATOM | 6024 | CB | ILE | D | 140 | 58.886 | 62.781 | 30.369 | 1.00 | 52.71 | 6 |
| | ATOM | 6025 | CG2 | ILE | D | 140 | 58.303 | 62.478 | 31.748 | 1.00 | 53.74 | 6 |
| | ATOM | 6026 | CG1 | ILE | D | 140 | 58.387 | 64.171 | 30.003 | 1.00 | 52.18 | 6 |
| 60 | ATOM | 6027 | CD1 | ILE | D | 140 | 56.892 | 64.354 | 30.322 | 1.00 | 51.22 | 6 |
| | ATOM | 6028 | C | ILE | D | 140 | 61.078 | 63.251 | 29.123 | 1.00 | 50.75 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 6029 | O | ILE | D | 140 | 61.189 | 64.451 | 28.918 | 1.00 | 50.51 | 8 |
| | ATOM | 6030 | N | GLY | D | 141 | 61.511 | 62.340 | 28.258 | 1.00 | 48.91 | 7 |
| | ATOM | 6031 | CA | GLY | D | 141 | 62.112 | 62.735 | 26.997 | 1.00 | 48.03 | 6 |
| | ATOM | 6032 | C | GLY | D | 141 | 62.036 | 61.611 | 25.983 | 1.00 | 47.81 | 6 |
| 5 | ATOM | 6033 | O | GLY | D | 141 | 61.636 | 60.511 | 26.340 | 1.00 | 50.42 | 8 |
| | ATOM | 6034 | N | SER | D | 142 | 62.405 | 61.865 | 24.729 | 1.00 | 45.08 | 7 |
| | ATOM | 6035 | CA | SER | D | 142 | 62.364 | 60.824 | 23.713 | 1.00 | 42.21 | 6 |
| | ATOM | 6036 | CB | SER | D | 142 | 62.872 | 61.334 | 22.376 | 1.00 | 43.40 | 6 |
| | ATOM | 6037 | OG | SER | D | 142 | 63.079 | 60.255 | 21.482 | 1.00 | 43.21 | 8 |
| 10 | ATOM | 6038 | C | SER | D | 142 | 63.194 | 59.630 | 24.126 | 1.00 | 44.37 | 6 |
| | ATOM | 6039 | O | SER | D | 142 | 64.284 | 59.758 | 24.688 | 1.00 | 45.99 | 8 |
| | ATOM | 6040 | N | TRP | D | 143 | 62.673 | 58.452 | 23.825 | 1.00 | 46.12 | 7 |
| | ATOM | 6041 | CA | TRP | D | 143 | 63.338 | 57.222 | 24.196 | 1.00 | 45.24 | 6 |
| | ATOM | 6042 | CB | TRP | D | 143 | 62.300 | 56.121 | 24.425 | 1.00 | 42.93 | 6 |
| 15 | ATOM | 6043 | CG | TRP | D | 143 | 62.872 | 54.893 | 25.051 | 1.00 | 39.90 | 6 |
| | ATOM | 6044 | CD2 | TRP | D | 143 | 63.244 | 54.737 | 26.418 | 1.00 | 37.42 | 6 |
| | ATOM | 6045 | CE2 | TRP | D | 143 | 63.740 | 53.425 | 26.567 | 1.00 | 37.64 | 6 |
| | ATOM | 6046 | CE3 | TRP | D | 143 | 63.204 | 55.581 | 27.536 | 1.00 | 35.75 | 6 |
| | ATOM | 6047 | CD1 | TRP | D | 143 | 63.154 | 53.702 | 24.436 | 1.00 | 40.17 | 6 |
| 20 | ATOM | 6048 | NE1 | TRP | D | 143 | 63.676 | 52.817 | 25.341 | 1.00 | 38.55 | 7 |
| | ATOM | 6049 | CZ2 | TRP | D | 143 | 64.187 | 52.935 | 27.788 | 1.00 | 38.02 | 6 |
| | ATOM | 6050 | CZ3 | TRP | D | 143 | 63.647 | 55.100 | 28.741 | 1.00 | 36.62 | 6 |
| | ATOM | 6051 | CH2 | TRP | D | 143 | 64.133 | 53.784 | 28.863 | 1.00 | 39.07 | 6 |
| | ATOM | 6052 | C | TRP | D | 143 | 64.348 | 56.758 | 23.170 | 1.00 | 46.24 | 6 |
| 25 | ATOM | 6053 | O | TRP | D | 143 | 65.328 | 56.109 | 23.509 | 1.00 | 48.11 | 8 |
| | ATOM | 6054 | N | THR | D | 144 | 64.124 | 57.080 | 21.910 | 1.00 | 45.62 | 7 |
| | ATOM | 6055 | CA | THR | D | 144 | 65.047 | 56.616 | 20.894 | 1.00 | 44.68 | 6 |
| | ATOM | 6056 | CB | THR | D | 144 | 64.336 | 55.633 | 19.955 | 1.00 | 44.87 | 6 |
| | ATOM | 6057 | OG1 | THR | D | 144 | 63.155 | 56.242 | 19.421 | 1.00 | 41.93 | 8 |
| 30 | ATOM | 6058 | CG2 | THR | D | 144 | 63.931 | 54.394 | 20.720 | 1.00 | 44.03 | 6 |
| | ATOM | 6059 | C | THR | D | 144 | 65.703 | 57.710 | 20.075 | 1.00 | 46.21 | 6 |
| | ATOM | 6060 | O | THR | D | 144 | 66.662 | 57.452 | 19.366 | 1.00 | 47.29 | 8 |
| | ATOM | 6061 | N | HIS | D | 145 | 65.198 | 58.931 | 20.173 | 1.00 | 47.13 | 7 |
| | ATOM | 6062 | CA | HIS | D | 145 | 65.772 | 60.021 | 19.403 | 1.00 | 50.18 | 6 |
| 35 | ATOM | 6063 | CB | HIS | D | 145 | 64.672 | 60.793 | 18.679 | 1.00 | 50.55 | 6 |
| | ATOM | 6064 | CG | HIS | D | 145 | 63.961 | 59.997 | 17.630 | 1.00 | 52.45 | 6 |
| | ATOM | 6065 | CD2 | HIS | D | 145 | 64.369 | 59.558 | 16.416 | 1.00 | 51.92 | 6 |
| | ATOM | 6066 | ND1 | HIS | D | 145 | 62.652 | 59.589 | 17.765 | 1.00 | 50.59 | 7 |
| | ATOM | 6067 | CE1 | HIS | D | 145 | 62.282 | 58.936 | 16.679 | 1.00 | 51.27 | 6 |
| 40 | ATOM | 6068 | NE2 | HIS | D | 145 | 63.305 | 58.902 | 15.844 | 1.00 | 52.81 | 7 |
| | ATOM | 6069 | C | HIS | D | 145 | 66.611 | 60.990 | 20.241 | 1.00 | 52.96 | 6 |
| | ATOM | 6070 | O | HIS | D | 145 | 66.147 | 61.554 | 21.236 | 1.00 | 51.74 | 8 |
| | ATOM | 6071 | N | HIS | D | 146 | 67.856 | 61.179 | 19.828 | 1.00 | 53.81 | 7 |
| | ATOM | 6072 | CA | HIS | D | 146 | 68.748 | 62.081 | 20.532 | 1.00 | 55.05 | 6 |
| 45 | ATOM | 6073 | CB | HIS | D | 146 | 70.205 | 61.691 | 20.267 | 1.00 | 53.71 | 6 |
| | ATOM | 6074 | CG | HIS | D | 146 | 70.555 | 61.617 | 18.816 | 1.00 | 52.77 | 6 |
| | ATOM | 6075 | CD2 | HIS | D | 146 | 70.425 | 62.526 | 17.821 | 1.00 | 53.89 | 6 |
| | ATOM | 6076 | ND1 | HIS | D | 146 | 71.083 | 60.487 | 18.236 | 1.00 | 49.45 | 7 |
| | ATOM | 6077 | CE1 | HIS | D | 146 | 71.261 | 60.700 | 16.945 | 1.00 | 49.76 | 6 |
| 50 | ATOM | 6078 | NE2 | HIS | D | 146 | 70.869 | 61.929 | 16.667 | 1.00 | 51.93 | 7 |
| | ATOM | 6079 | C | HIS | D | 146 | 68.489 | 63.521 | 20.094 | 1.00 | 56.51 | 6 |
| | ATOM | 6080 | O | HIS | D | 146 | 67.682 | 63.770 | 19.185 | 1.00 | 58.53 | 8 |
| | ATOM | 6081 | N | SER | D | 147 | 69.190 | 64.455 | 20.738 | 1.00 | 57.97 | 7 |
| | ATOM | 6082 | CA | SER | D | 147 | 69.054 | 65.902 | 20.497 | 1.00 | 58.69 | 6 |
| 55 | ATOM | 6083 | CB | SER | D | 147 | 70.097 | 66.646 | 21.332 | 1.00 | 58.36 | 6 |
| | ATOM | 6084 | OG | SER | D | 147 | 71.365 | 66.032 | 21.179 | 1.00 | 58.90 | 8 |
| | ATOM | 6085 | C | SER | D | 147 | 69.114 | 66.404 | 19.049 | 1.00 | 57.67 | 6 |
| | ATOM | 6086 | O | SER | D | 147 | 68.570 | 67.470 | 18.727 | 1.00 | 55.79 | 8 |
| | ATOM | 6087 | N | ARG | D | 148 | 69.768 | 65.647 | 18.180 | 1.00 | 57.54 | 7 |
| 60 | ATOM | 6088 | CA | ARG | D | 148 | 69.878 | 66.061 | 16.790 | 1.00 | 59.37 | 6 |
| | ATOM | 6089 | CB | ARG | D | 148 | 71.054 | 65.340 | 16.126 | 1.00 | 64.67 | 6 |

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| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 6090 | CG | ARG | D | 148 | 72.382 | 65.498 | 16.869 | 1.00 | 73.01 | 6 |
| | ATOM | 6091 | CD | ARG | D | 148 | 73.494 | 64.621 | 16.270 | 1.00 | 79.78 | 6 |
| | ATOM | 6092 | NE | ARG | D | 148 | 74.652 | 64.495 | 17.172 | 1.00 | 86.45 | 7 |
| | ATOM | 6093 | CZ | ARG | D | 148 | 75.435 | 65.508 | 17.558 | 1.00 | 88.85 | 6 |
| 5 | ATOM | 6094 | NH1 | ARG | D | 148 | 75.200 | 66.749 | 17.126 | 1.00 | 90.23 | 7 |
| | ATOM | 6095 | NH2 | ARG | D | 148 | 76.462 | 65.284 | 18.381 | 1.00 | 89.74 | 7 |
| | ATOM | 6096 | C | ARG | D | 148 | 68.603 | 65.790 | 16.001 | 1.00 | 58.14 | 6 |
| | ATOM | 6097 | O | ARG | D | 148 | 68.406 | 66.351 | 14.921 | 1.00 | 57.28 | 8 |
| | ATOM | 6098 | N | GLU | D | 149 | 67.737 | 64.932 | 16.546 | 1.00 | 58.44 | 7 |
| 10 | ATOM | 6099 | CA | GLU | D | 149 | 66.488 | 64.555 | 15.881 | 1.00 | 54.51 | 6 |
| | ATOM | 6100 | CB | GLU | D | 149 | 66.394 | 63.030 | 15.787 | 1.00 | 54.24 | 6 |
| | ATOM | 6101 | CG | GLU | D | 149 | 67.744 | 62.384 | 15.474 | 1.00 | 56.46 | 6 |
| | ATOM | 6102 | CD | GLU | D | 149 | 67.687 | 60.886 | 15.343 | 1.00 | 57.56 | 6 |
| | ATOM | 6103 | OE1 | GLU | D | 149 | 67.015 | 60.226 | 16.171 | 1.00 | 60.61 | 8 |
| 15 | ATOM | 6104 | OE2 | GLU | D | 149 | 68.336 | 60.365 | 14.415 | 1.00 | 56.79 | 8 |
| | ATOM | 6105 | C | GLU | D | 149 | 65.315 | 65.123 | 16.638 | 1.00 | 51.56 | 6 |
| | ATOM | 6106 | O | GLU | D | 149 | 64.396 | 65.667 | 16.050 | 1.00 | 48.50 | 8 |
| | ATOM | 6107 | N | ILE | D | 150 | 65.355 | 65.002 | 17.954 | 1.00 | 51.48 | 7 |
| | ATOM | 6108 | CA | ILE | D | 150 | 64.284 | 65.533 | 18.783 | 1.00 | 53.11 | 6 |
| 20 | ATOM | 6109 | CB | ILE | D | 150 | 63.382 | 64.424 | 19.410 | 1.00 | 55.50 | 6 |
| | ATOM | 6110 | CG2 | ILE | D | 150 | 62.530 | 65.013 | 20.542 | 1.00 | 52.41 | 6 |
| | ATOM | 6111 | CG1 | ILE | D | 150 | 62.440 | 63.830 | 18.352 | 1.00 | 55.09 | 6 |
| | ATOM | 6112 | CD1 | ILE | D | 150 | 61.549 | 62.728 | 18.884 | 1.00 | 53.30 | 6 |
| | ATOM | 6113 | C | ILE | D | 150 | 64.841 | 66.339 | 19.925 | 1.00 | 54.06 | 6 |
| 25 | ATOM | 6114 | O | ILE | D | 150 | 65.809 | 65.944 | 20.573 | 1.00 | 49.46 | 8 |
| | ATOM | 6115 | N | SER | D | 151 | 64.199 | 67.474 | 20.162 | 1.00 | 55.80 | 7 |
| | ATOM | 6116 | CA | SER | D | 151 | 64.570 | 68.365 | 21.245 | 1.00 | 57.52 | 6 |
| | ATOM | 6117 | CB | SER | D | 151 | 65.190 | 69.660 | 20.688 | 1.00 | 59.00 | 6 |
| | ATOM | 6118 | OG | SER | D | 151 | 64.256 | 70.404 | 19.906 | 1.00 | 62.67 | 8 |
| 30 | ATOM | 6119 | C | SER | D | 151 | 63.269 | 68.663 | 21.989 | 1.00 | 57.81 | 6 |
| | ATOM | 6120 | O | SER | D | 151 | 62.241 | 68.932 | 21.373 | 1.00 | 55.28 | 8 |
| | ATOM | 6121 | N | VAL | D | 152 | 63.315 | 68.592 | 23.312 | 1.00 | 59.48 | 7 |
| | ATOM | 6122 | CA | VAL | D | 152 | 62.142 | 68.851 | 24.132 | 1.00 | 62.33 | 6 |
| | ATOM | 6123 | CB | VAL | D | 152 | 61.940 | 67.742 | 25.188 | 1.00 | 63.11 | 6 |
| 35 | ATOM | 6124 | CG1 | VAL | D | 152 | 61.945 | 66.373 | 24.511 | 1.00 | 63.08 | 6 |
| | ATOM | 6125 | CG2 | VAL | D | 152 | 63.038 | 67.821 | 26.259 | 1.00 | 61.64 | 6 |
| | ATOM | 6126 | C | VAL | D | 152 | 62.350 | 70.167 | 24.854 | 1.00 | 63.67 | 6 |
| | ATOM | 6127 | O | VAL | D | 152 | 63.478 | 70.496 | 25.231 | 1.00 | 63.11 | 8 |
| | ATOM | 6128 | N | ASP | D | 153 | 61.266 | 70.909 | 25.070 | 1.00 | 65.73 | 7 |
| 40 | ATOM | 6129 | CA | ASP | D | 153 | 61.365 | 72.206 | 25.740 | 1.00 | 68.62 | 6 |
| | ATOM | 6130 | CB | ASP | D | 153 | 61.524 | 73.296 | 24.680 | 1.00 | 70.73 | 6 |
| | ATOM | 6131 | CG | ASP | D | 153 | 62.698 | 73.023 | 23.733 | 1.00 | 74.59 | 6 |
| | ATOM | 6132 | OD1 | ASP | D | 153 | 63.854 | 73.332 | 24.118 | 1.00 | 73.93 | 8 |
| | ATOM | 6133 | OD2 | ASP | D | 153 | 62.473 | 72.483 | 22.612 | 1.00 | 76.61 | 8 |
| 45 | ATOM | 6134 | C | ASP | D | 153 | 60.144 | 72.513 | 26.601 | 1.00 | 69.92 | 6 |
| | ATOM | 6135 | O | ASP | D | 153 | 59.022 | 72.176 | 26.227 | 1.00 | 71.07 | 8 |
| | ATOM | 6136 | N | PRO | D | 154 | 60.345 | 73.139 | 27.778 | 1.00 | 71.13 | 7 |
| | ATOM | 6137 | CD | PRO | D | 154 | 61.609 | 73.207 | 28.536 | 1.00 | 70.02 | 6 |
| | ATOM | 6138 | CA | PRO | D | 154 | 59.199 | 73.471 | 28.645 | 1.00 | 72.68 | 6 |
| 50 | ATOM | 6139 | CB | PRO | D | 154 | 59.863 | 73.882 | 29.955 | 1.00 | 71.74 | 6 |
| | ATOM | 6140 | CG | PRO | D | 154 | 61.135 | 73.062 | 29.962 | 1.00 | 70.60 | 6 |
| | ATOM | 6141 | C | PRO | D | 154 | 58.374 | 74.609 | 28.030 | 1.00 | 75.79 | 6 |
| | ATOM | 6142 | O | PRO | D | 154 | 58.732 | 75.140 | 26.983 | 1.00 | 76.11 | 8 |
| | ATOM | 6143 | N | THR | D | 155 | 57.286 | 75.001 | 28.686 | 1.00 | 80.37 | 7 |
| 55 | ATOM | 6144 | CA | THR | D | 155 | 56.419 | 76.060 | 28.148 | 1.00 | 84.32 | 6 |
| | ATOM | 6145 | CB | THR | D | 155 | 55.208 | 75.436 | 27.393 | 1.00 | 84.09 | 6 |
| | ATOM | 6146 | OG1 | THR | D | 155 | 54.342 | 74.785 | 28.337 | 1.00 | 83.35 | 8 |
| | ATOM | 6147 | CG2 | THR | D | 155 | 55.685 | 74.412 | 26.360 | 1.00 | 83.23 | 6 |
| | ATOM | 6148 | C | THR | D | 155 | 55.861 | 77.068 | 29.184 | 1.00 | 88.09 | 6 |
| 60 | ATOM | 6149 | O | THR | D | 155 | 56.510 | 77.366 | 30.211 | 1.00 | 88.59 | 8 |
| | ATOM | 6150 | N | THR | D | 156 | 54.654 | 77.578 | 28.886 | 1.00 | 91.07 | 7 |

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|----|------|------|-----|-----------|--------|--------|--------|------|--------|---|
| 5 | ATOM | 6151 | CA | THR D 156 | 53.911 | 78.559 | 29.705 | 1.00 | 93.25 | 6 |
| | ATOM | 6152 | CB | THR D 156 | 52.372 | 78.483 | 29.424 | 1.00 | 94.48 | 6 |
| | ATOM | 6153 | OG1 | THR D 156 | 52.115 | 78.686 | 28.019 | 1.00 | 94.94 | 8 |
| | ATOM | 6154 | CG2 | THR D 156 | 51.619 | 79.546 | 30.255 | 1.00 | 93.74 | 6 |
| | ATOM | 6155 | C | THR D 156 | 54.104 | 78.445 | 31.220 | 1.00 | 94.44 | 6 |
| 10 | ATOM | 6156 | O | THR D 156 | 53.471 | 77.615 | 31.898 | 1.00 | 93.56 | 8 |
| | ATOM | 6157 | N | GLU D 157 | 54.955 | 79.314 | 31.750 | 1.00 | 96.79 | 7 |
| | ATOM | 6158 | CA | GLU D 157 | 55.252 | 79.320 | 33.183 | 1.00 | 99.37 | 6 |
| | ATOM | 6159 | CB | GLU D 157 | 56.670 | 79.865 | 33.416 | 1.00 | 100.34 | 6 |
| | ATOM | 6160 | CG | GLU D 157 | 57.701 | 79.333 | 32.426 | 1.00 | 102.84 | 6 |
| 15 | ATOM | 6161 | CD | GLU D 157 | 59.086 | 79.955 | 32.629 | 1.00 | 104.89 | 6 |
| | ATOM | 6162 | OE1 | GLU D 157 | 59.179 | 81.213 | 32.700 | 1.00 | 104.68 | 8 |
| | ATOM | 6163 | OE2 | GLU D 157 | 60.085 | 79.189 | 32.707 | 1.00 | 105.54 | 8 |
| | ATOM | 6164 | C | GLU D 157 | 54.237 | 80.165 | 33.967 | 1.00 | 99.49 | 6 |
| | ATOM | 6165 | O | GLU D 157 | 54.273 | 80.216 | 35.210 | 1.00 | 100.21 | 8 |
| 20 | ATOM | 6166 | N | ASN D 158 | 53.336 | 80.828 | 33.248 | 1.00 | 98.56 | 7 |
| | ATOM | 6167 | CA | ASN D 158 | 52.340 | 81.657 | 33.911 | 1.00 | 98.16 | 6 |
| | ATOM | 6168 | CB | ASN D 158 | 51.632 | 82.550 | 32.894 | 1.00 | 100.26 | 6 |
| | ATOM | 6169 | CG | ASN D 158 | 52.610 | 83.378 | 32.064 | 1.00 | 102.10 | 6 |
| | ATOM | 6170 | OD1 | ASN D 158 | 53.425 | 84.153 | 32.607 | 1.00 | 101.77 | 8 |
| 25 | ATOM | 6171 | ND2 | ASN D 158 | 52.533 | 83.221 | 30.735 | 1.00 | 102.21 | 7 |
| | ATOM | 6172 | C | ASN D 158 | 51.313 | 80.786 | 34.613 | 1.00 | 96.52 | 6 |
| | ATOM | 6173 | O | ASN D 158 | 51.475 | 80.452 | 35.797 | 1.00 | 96.76 | 8 |
| | ATOM | 6174 | N | SER D 159 | 50.257 | 80.447 | 33.864 | 1.00 | 94.02 | 7 |
| | ATOM | 6175 | CA | SER D 159 | 49.142 | 79.599 | 34.313 | 1.00 | 90.18 | 6 |
| 30 | ATOM | 6176 | CB | SER D 159 | 48.996 | 78.422 | 33.331 | 1.00 | 90.25 | 6 |
| | ATOM | 6177 | OG | SER D 159 | 50.277 | 77.932 | 32.940 | 1.00 | 90.19 | 8 |
| | ATOM | 6178 | C | SER D 159 | 49.254 | 79.071 | 35.751 | 1.00 | 87.40 | 6 |
| | ATOM | 6179 | O | SER D 159 | 50.208 | 78.372 | 36.094 | 1.00 | 87.99 | 8 |
| | ATOM | 6180 | N | ASP D 160 | 48.282 | 79.408 | 36.594 | 1.00 | 83.57 | 7 |
| 35 | ATOM | 6181 | CA | ASP D 160 | 48.300 | 78.947 | 37.984 | 1.00 | 79.69 | 6 |
| | ATOM | 6182 | CB | ASP D 160 | 46.950 | 79.189 | 38.660 | 1.00 | 79.26 | 6 |
| | ATOM | 6183 | CG | ASP D 160 | 46.902 | 78.632 | 40.079 | 1.00 | 79.02 | 6 |
| | ATOM | 6184 | OD1 | ASP D 160 | 45.785 | 78.385 | 40.596 | 1.00 | 78.94 | 8 |
| | ATOM | 6185 | OD2 | ASP D 160 | 47.987 | 78.446 | 40.679 | 1.00 | 77.43 | 8 |
| 40 | ATOM | 6186 | C | ASP D 160 | 48.579 | 77.453 | 37.995 | 1.00 | 77.55 | 6 |
| | ATOM | 6187 | O | ASP D 160 | 47.797 | 76.670 | 37.429 | 1.00 | 77.70 | 8 |
| | ATOM | 6188 | N | ASP D 161 | 49.676 | 77.062 | 38.646 | 1.00 | 74.02 | 7 |
| | ATOM | 6189 | CA | ASP D 161 | 50.070 | 75.657 | 38.719 | 1.00 | 69.51 | 6 |
| | ATOM | 6190 | CB | ASP D 161 | 51.277 | 75.466 | 39.642 | 1.00 | 68.24 | 6 |
| 45 | ATOM | 6191 | CG | ASP D 161 | 52.556 | 76.004 | 39.050 | 1.00 | 67.15 | 6 |
| | ATOM | 6192 | OD1 | ASP D 161 | 52.734 | 75.886 | 37.827 | 1.00 | 67.47 | 8 |
| | ATOM | 6193 | OD2 | ASP D 161 | 53.397 | 76.536 | 39.803 | 1.00 | 70.25 | 8 |
| | ATOM | 6194 | C | ASP D 161 | 48.972 | 74.697 | 39.147 | 1.00 | 67.31 | 6 |
| | ATOM | 6195 | O | ASP D 161 | 49.071 | 73.497 | 38.890 | 1.00 | 68.61 | 8 |
| 50 | ATOM | 6196 | N | SER D 162 | 47.924 | 75.191 | 39.788 | 1.00 | 64.39 | 7 |
| | ATOM | 6197 | CA | SER D 162 | 46.871 | 74.280 | 40.210 | 1.00 | 63.54 | 6 |
| | ATOM | 6198 | CB | SER D 162 | 46.897 | 74.097 | 41.736 | 1.00 | 63.26 | 6 |
| | ATOM | 6199 | OG | SER D 162 | 46.555 | 75.286 | 42.417 | 1.00 | 65.64 | 8 |
| | ATOM | 6200 | C | SER D 162 | 45.494 | 74.722 | 39.761 | 1.00 | 62.73 | 6 |
| 55 | ATOM | 6201 | O | SER D 162 | 44.490 | 74.439 | 40.425 | 1.00 | 60.67 | 8 |
| | ATOM | 6202 | N | GLU D 163 | 45.435 | 75.400 | 38.620 | 1.00 | 63.28 | 7 |
| | ATOM | 6203 | CA | GLU D 163 | 44.149 | 75.861 | 38.139 | 1.00 | 66.60 | 6 |
| | ATOM | 6204 | CB | GLU D 163 | 44.325 | 76.984 | 37.105 | 1.00 | 69.72 | 6 |
| | ATOM | 6205 | CG | GLU D 163 | 44.576 | 76.546 | 35.681 | 1.00 | 72.12 | 6 |
| 60 | ATOM | 6206 | CD | GLU D 163 | 44.506 | 77.720 | 34.698 | 1.00 | 74.42 | 6 |
| | ATOM | 6207 | OE1 | GLU D 163 | 45.442 | 78.557 | 34.703 | 1.00 | 75.59 | 8 |
| | ATOM | 6208 | OE2 | GLU D 163 | 43.510 | 77.808 | 33.932 | 1.00 | 73.89 | 8 |
| | ATOM | 6209 | C | GLU D 163 | 43.310 | 74.712 | 37.572 | 1.00 | 65.25 | 6 |
| | ATOM | 6210 | O | GLU D 163 | 42.126 | 74.885 | 37.264 | 1.00 | 65.73 | 8 |
| | ATOM | 6211 | N | TYR D 164 | 43.926 | 73.539 | 37.448 | 1.00 | 64.10 | 7 |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 6212 | CA TYR D 164 | 43.236 | 72.353 | 36.946 | 1.00 | 61.14 | 6 | |
| | ATOM | 6213 | CB TYR D 164 | 43.901 | 71.828 | 35.675 | 1.00 | 62.34 | 6 | |
| | ATOM | 6214 | CG TYR D 164 | 43.794 | 72.756 | 34.501 | 1.00 | 62.07 | 6 | |
| | ATOM | 6215 | CD1 TYR D 164 | 44.937 | 73.264 | 33.887 | 1.00 | 62.29 | 6 | |
| | ATOM | 6216 | CE1 TYR D 164 | 44.846 | 74.152 | 32.813 | 1.00 | 64.14 | 6 | |
| | ATOM | 6217 | CD2 TYR D 164 | 42.547 | 73.151 | 34.016 | 1.00 | 63.36 | 6 | |
| | ATOM | 6218 | CE2 TYR D 164 | 42.438 | 74.038 | 32.940 | 1.00 | 65.18 | 6 | |
| | ATOM | 6219 | CZ TYR D 164 | 43.594 | 74.536 | 32.337 | 1.00 | 65.18 | 6 | |
| 10 | ATOM | 6220 | OH TYR D 164 | 43.495 | 75.380 | 31.240 | 1.00 | 65.32 | 8 | |
| | ATOM | 6221 | C TYR D 164 | 43.257 | 71.263 | 38.000 | 1.00 | 59.77 | 6 | |
| | ATOM | 6222 | O TYR D 164 | 42.602 | 70.231 | 37.853 | 1.00 | 59.16 | 8 | |
| | ATOM | 6223 | N PHE D 165 | 44.008 | 71.497 | 39.068 | 1.00 | 57.70 | 7 | |
| 15 | ATOM | 6224 | CA PHE D 165 | 44.113 | 70.518 | 40.143 | 1.00 | 56.00 | 6 | |
| | ATOM | 6225 | CB PHE D 165 | 45.105 | 70.988 | 41.202 | 1.00 | 53.27 | 6 | |
| | ATOM | 6226 | CG PHE D 165 | 45.635 | 69.885 | 42.053 | 1.00 | 51.93 | 6 | |
| | ATOM | 6227 | CD1 PHE D 165 | 46.436 | 68.891 | 41.502 | 1.00 | 50.62 | 6 | |
| | ATOM | 6228 | CD2 PHE D 165 | 45.326 | 69.820 | 43.398 | 1.00 | 52.41 | 6 | |
| | ATOM | 6229 | CE1 PHE D 165 | 46.922 | 67.845 | 42.283 | 1.00 | 49.13 | 6 | |
| 20 | ATOM | 6230 | CE2 PHE D 165 | 45.807 | 68.777 | 44.188 | 1.00 | 52.20 | 6 | |
| | ATOM | 6231 | CZ PHE D 165 | 46.608 | 67.788 | 43.624 | 1.00 | 51.98 | 6 | |
| | ATOM | 6232 | C PHE D 165 | 42.773 | 70.241 | 40.801 | 1.00 | 55.90 | 6 | |
| | ATOM | 6233 | O PHE D 165 | 41.970 | 71.149 | 41.005 | 1.00 | 56.82 | 8 | |
| 25 | ATOM | 6234 | N SER D 166 | 42.524 | 68.980 | 41.126 | 1.00 | 55.56 | 7 | |
| | ATOM | 6235 | CA SER D 166 | 41.273 | 68.627 | 41.771 | 1.00 | 55.90 | 6 | |
| | ATOM | 6236 | CB SER D 166 | 41.115 | 67.117 | 41.887 | 1.00 | 55.69 | 6 | |
| | ATOM | 6237 | OG SER D 166 | 39.855 | 66.799 | 42.457 | 1.00 | 55.69 | 8 | |
| | ATOM | 6238 | C SER D 166 | 41.280 | 69.229 | 43.158 | 1.00 | 56.73 | 6 | |
| | ATOM | 6239 | O SER D 166 | 42.315 | 69.229 | 43.839 | 1.00 | 56.74 | 8 | |
| 30 | ATOM | 6240 | N GLN D 167 | 40.121 | 69.729 | 43.578 | 1.00 | 57.58 | 7 | |
| | ATOM | 6241 | CA GLN D 167 | 39.999 | 70.353 | 44.892 | 1.00 | 57.81 | 6 | |
| | ATOM | 6242 | CB GLN D 167 | 38.867 | 71.383 | 44.885 | 1.00 | 59.24 | 6 | |
| | ATOM | 6243 | CG GLN D 167 | 37.541 | 70.794 | 44.439 | 1.00 | 63.59 | 6 | |
| | ATOM | 6244 | CD GLN D 167 | 36.485 | 71.854 | 44.107 | 1.00 | 65.57 | 6 | |
| | ATOM | 6245 | OE1 GLN D 167 | 36.054 | 72.607 | 44.979 | 1.00 | 65.98 | 8 | |
| 35 | ATOM | 6246 | NE2 GLN D 167 | 36.067 | 71.909 | 42.831 | 1.00 | 65.54 | 7 | |
| | ATOM | 6247 | C GLN D 167 | 39.752 | 69.328 | 45.977 | 1.00 | 56.65 | 6 | |
| | ATOM | 6248 | O GLN D 167 | 39.990 | 69.598 | 47.151 | 1.00 | 56.95 | 8 | |
| | ATOM | 6249 | N TYR D 168 | 39.293 | 68.145 | 45.586 | 1.00 | 56.16 | 7 | |
| 40 | ATOM | 6250 | CA TYR D 168 | 39.014 | 67.091 | 46.556 | 1.00 | 53.65 | 6 | |
| | ATOM | 6251 | CB TYR D 168 | 37.798 | 66.297 | 46.096 | 1.00 | 54.14 | 6 | |
| | ATOM | 6252 | CG TYR D 168 | 36.675 | 67.217 | 45.707 | 1.00 | 53.82 | 6 | |
| | ATOM | 6253 | CD1 TYR D 168 | 36.446 | 67.545 | 44.371 | 1.00 | 53.19 | 6 | |
| | ATOM | 6254 | CE1 TYR D 168 | 35.445 | 68.454 | 44.020 | 1.00 | 54.20 | 6 | |
| | ATOM | 6255 | CD2 TYR D 168 | 35.880 | 67.816 | 46.681 | 1.00 | 52.39 | 6 | |
| 45 | ATOM | 6256 | CE2 TYR D 168 | 34.881 | 68.722 | 46.342 | 1.00 | 52.03 | 6 | |
| | ATOM | 6257 | CZ TYR D 168 | 34.670 | 69.035 | 45.016 | 1.00 | 53.04 | 6 | |
| | ATOM | 6258 | OH TYR D 168 | 33.683 | 69.917 | 44.689 | 1.00 | 53.97 | 8 | |
| | ATOM | 6259 | C TYR D 168 | 40.181 | 66.162 | 46.851 | 1.00 | 52.39 | 6 | |
| 50 | ATOM | 6260 | O TYR D 168 | 40.025 | 65.185 | 47.575 | 1.00 | 53.02 | 8 | |
| | ATOM | 6261 | N SER D 169 | 41.347 | 66.479 | 46.299 | 1.00 | 51.48 | 7 | |
| | ATOM | 6262 | CA SER D 169 | 42.543 | 65.686 | 46.513 | 1.00 | 51.84 | 6 | |
| | ATOM | 6263 | CB SER D 169 | 43.664 | 66.151 | 45.584 | 1.00 | 52.14 | 6 | |
| | ATOM | 6264 | OG SER D 169 | 44.878 | 65.483 | 45.881 | 1.00 | 50.95 | 8 | |
| | ATOM | 6265 | C SER D 169 | 43.001 | 65.828 | 47.953 | 1.00 | 53.72 | 6 | |
| 55 | ATOM | 6266 | O SER D 169 | 42.832 | 66.880 | 48.570 | 1.00 | 51.67 | 8 | |
| | ATOM | 6267 | N ARG D 170 | 43.583 | 64.761 | 48.487 | 1.00 | 54.84 | 7 | |
| | ATOM | 6268 | CA ARG D 170 | 44.079 | 64.778 | 49.850 | 1.00 | 54.97 | 6 | |
| | ATOM | 6269 | CB ARG D 170 | 44.460 | 63.366 | 50.297 | 1.00 | 54.29 | 6 | |
| 60 | ATOM | 6270 | CG ARG D 170 | 43.369 | 62.647 | 51.081 | 1.00 | 57.60 | 6 | |
| | ATOM | 6271 | CD ARG D 170 | 43.436 | 61.124 | 50.955 | 1.00 | 58.91 | 6 | |
| | ATOM | 6272 | NE ARG D 170 | 44.726 | 60.543 | 51.323 | 1.00 | 61.45 | 7 | |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 6273 | CZ | ARG D 170 | 45.504 | 59.853 | 50.483 | 1.00 | 64.08 | 6 |
| | ATOM | 6274 | NH1 | ARG D 170 | 45.140 | 59.656 | 49.220 | 1.00 | 60.98 | 7 |
| | ATOM | 6275 | NH2 | ARG D 170 | 46.649 | 59.334 | 50.906 | 1.00 | 64.65 | 7 |
| | ATOM | 6276 | C | ARG D 170 | 45.293 | 65.683 | 49.928 | 1.00 | 56.57 | 6 |
| | ATOM | 6277 | O | ARG D 170 | 45.719 | 66.078 | 51.022 | 1.00 | 59.46 | 8 |
| 10 | ATOM | 6278 | N | PHE D 171 | 45.842 | 66.033 | 48.770 | 1.00 | 55.26 | 7 |
| | ATOM | 6279 | CA | PHE D 171 | 47.034 | 66.864 | 48.739 | 1.00 | 54.09 | 6 |
| | ATOM | 6280 | CB | PHE D 171 | 48.172 | 66.094 | 48.070 | 1.00 | 53.61 | 6 |
| | ATOM | 6281 | CG | PHE D 171 | 48.319 | 64.688 | 48.585 | 1.00 | 54.38 | 6 |
| | ATOM | 6282 | CD1 | PHE D 171 | 47.427 | 63.698 | 48.191 | 1.00 | 55.63 | 6 |
| 15 | ATOM | 6283 | CD2 | PHE D 171 | 49.315 | 64.364 | 49.498 | 1.00 | 54.14 | 6 |
| | ATOM | 6284 | CE1 | PHE D 171 | 47.521 | 62.415 | 48.694 | 1.00 | 54.27 | 6 |
| | ATOM | 6285 | CE2 | PHE D 171 | 49.414 | 63.078 | 50.008 | 1.00 | 54.92 | 6 |
| | ATOM | 6286 | CZ | PHE D 171 | 48.516 | 62.103 | 49.605 | 1.00 | 54.58 | 6 |
| | ATOM | 6287 | C | PHE D 171 | 46.821 | 68.195 | 48.049 | 1.00 | 53.25 | 6 |
| 20 | ATOM | 6288 | O | PHE D 171 | 45.759 | 68.457 | 47.500 | 1.00 | 52.23 | 8 |
| | ATOM | 6289 | N | GLU D 172 | 47.836 | 69.045 | 48.100 | 1.00 | 52.75 | 7 |
| | ATOM | 6290 | CA | GLU D 172 | 47.741 | 70.347 | 47.479 | 1.00 | 55.31 | 6 |
| | ATOM | 6291 | CB | GLU D 172 | 47.327 | 71.413 | 48.505 | 1.00 | 58.80 | 6 |
| | ATOM | 6292 | CG | GLU D 172 | 48.293 | 71.616 | 49.686 | 1.00 | 62.32 | 6 |
| 25 | ATOM | 6293 | CD | GLU D 172 | 47.773 | 72.633 | 50.693 | 1.00 | 64.33 | 6 |
| | ATOM | 6294 | OE1 | GLU D 172 | 47.132 | 73.617 | 50.251 | 1.00 | 64.06 | 8 |
| | ATOM | 6295 | OE2 | GLU D 172 | 48.012 | 72.456 | 51.915 | 1.00 | 65.29 | 8 |
| | ATOM | 6296 | C | GLU D 172 | 49.083 | 70.671 | 46.861 | 1.00 | 56.32 | 6 |
| | ATOM | 6297 | O | GLU D 172 | 50.115 | 70.122 | 47.265 | 1.00 | 54.59 | 8 |
| 30 | ATOM | 6298 | N | ILE D 173 | 49.063 | 71.550 | 45.864 | 1.00 | 56.82 | 7 |
| | ATOM | 6299 | CA | ILE D 173 | 50.286 | 71.928 | 45.171 | 1.00 | 57.96 | 6 |
| | ATOM | 6300 | CB | ILE D 173 | 50.062 | 72.033 | 43.644 | 1.00 | 57.06 | 6 |
| | ATOM | 6301 | CG2 | ILE D 173 | 51.332 | 72.535 | 42.959 | 1.00 | 56.84 | 6 |
| | ATOM | 6302 | CG1 | ILE D 173 | 49.663 | 70.675 | 43.080 | 1.00 | 55.34 | 6 |
| 35 | ATOM | 6303 | CD1 | ILE D 173 | 49.371 | 70.720 | 41.622 | 1.00 | 53.59 | 6 |
| | ATOM | 6304 | C | ILE D 173 | 50.848 | 73.250 | 45.653 | 1.00 | 59.20 | 6 |
| | ATOM | 6305 | O | ILE D 173 | 50.132 | 74.249 | 45.756 | 1.00 | 58.03 | 8 |
| | ATOM | 6306 | N | LEU D 174 | 52.140 | 73.251 | 45.949 | 1.00 | 60.22 | 7 |
| | ATOM | 6307 | CA | LEU D 174 | 52.784 | 74.473 | 46.394 | 1.00 | 61.88 | 6 |
| 40 | ATOM | 6308 | CB | LEU D 174 | 53.929 | 74.136 | 47.340 | 1.00 | 61.02 | 6 |
| | ATOM | 6309 | CG | LEU D 174 | 53.512 | 73.196 | 48.469 | 1.00 | 61.46 | 6 |
| | ATOM | 6310 | CD1 | LEU D 174 | 54.722 | 72.881 | 49.330 | 1.00 | 62.06 | 6 |
| | ATOM | 6311 | CD2 | LEU D 174 | 52.395 | 73.823 | 49.284 | 1.00 | 59.37 | 6 |
| | ATOM | 6312 | C | LEU D 174 | 53.302 | 75.193 | 45.151 | 1.00 | 63.17 | 6 |
| 45 | ATOM | 6313 | O | LEU D 174 | 52.979 | 76.357 | 44.899 | 1.00 | 63.68 | 8 |
| | ATOM | 6314 | N | ASP D 175 | 54.080 | 74.479 | 44.349 | 1.00 | 64.58 | 7 |
| | ATOM | 6315 | CA | ASP D 175 | 54.627 | 75.067 | 43.145 | 1.00 | 65.97 | 6 |
| | ATOM | 6316 | CB | ASP D 175 | 55.789 | 75.993 | 43.538 | 1.00 | 67.34 | 6 |
| | ATOM | 6317 | CG | ASP D 175 | 56.390 | 76.748 | 42.354 | 1.00 | 69.43 | 6 |
| 50 | ATOM | 6318 | OD1 | ASP D 175 | 55.636 | 77.413 | 41.584 | 1.00 | 69.68 | 8 |
| | ATOM | 6319 | OD2 | ASP D 175 | 57.635 | 76.685 | 42.214 | 1.00 | 69.28 | 8 |
| | ATOM | 6320 | C | ASP D 175 | 55.085 | 73.984 | 42.164 | 1.00 | 66.38 | 6 |
| | ATOM | 6321 | O | ASP D 175 | 55.380 | 72.846 | 42.561 | 1.00 | 66.58 | 8 |
| | ATOM | 6322 | N | VAL D 176 | 55.118 | 74.342 | 40.881 | 1.00 | 65.75 | 7 |
| 55 | ATOM | 6323 | CA | VAL D 176 | 55.536 | 73.436 | 39.831 | 1.00 | 65.19 | 6 |
| | ATOM | 6324 | CB | VAL D 176 | 54.330 | 72.945 | 38.992 | 1.00 | 64.89 | 6 |
| | ATOM | 6325 | CG1 | VAL D 176 | 54.818 | 72.085 | 37.811 | 1.00 | 64.67 | 6 |
| | ATOM | 6326 | CG2 | VAL D 176 | 53.382 | 72.145 | 39.865 | 1.00 | 65.95 | 6 |
| | ATOM | 6327 | C | VAL D 176 | 56.477 | 74.190 | 38.919 | 1.00 | 66.36 | 6 |
| 60 | ATOM | 6328 | O | VAL D 176 | 56.178 | 75.314 | 38.513 | 1.00 | 66.32 | 8 |
| | ATOM | 6329 | N | THR D 177 | 57.614 | 73.576 | 38.602 | 1.00 | 68.04 | 7 |
| | ATOM | 6330 | CA | THR D 177 | 58.598 | 74.184 | 37.708 | 1.00 | 69.05 | 6 |
| | ATOM | 6331 | CB | THR D 177 | 59.763 | 74.819 | 38.496 | 1.00 | 67.62 | 6 |
| | ATOM | 6332 | OG1 | THR D 177 | 60.349 | 73.843 | 39.370 | 1.00 | 63.42 | 8 |
| | ATOM | 6333 | CG2 | THR D 177 | 59.258 | 76.013 | 39.305 | 1.00 | 66.11 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 6334 | C | THR | D | 177 | 59.165 | 73.144 | 36.739 | 1.00 | 71.66 | 6 |
| | ATOM | 6335 | O | THR | D | 177 | 59.373 | 71.973 | 37.111 | 1.00 | 73.56 | 8 |
| | ATOM | 6336 | N | GLN | D | 178 | 59.417 | 73.568 | 35.501 | 1.00 | 71.95 | 7 |
| | ATOM | 6337 | CA | GLN | D | 178 | 59.941 | 72.667 | 34.488 | 1.00 | 72.06 | 6 |
| 5 | ATOM | 6338 | CB | GLN | D | 178 | 58.932 | 72.511 | 33.347 | 1.00 | 74.14 | 6 |
| | ATOM | 6339 | CG | GLN | D | 178 | 57.466 | 72.700 | 33.754 | 1.00 | 76.97 | 6 |
| | ATOM | 6340 | CD | GLN | D | 178 | 56.497 | 72.041 | 32.772 | 1.00 | 78.22 | 6 |
| | ATOM | 6341 | OE1 | GLN | D | 178 | 56.603 | 72.230 | 31.551 | 1.00 | 79.44 | 8 |
| | ATOM | 6342 | NE2 | GLN | D | 178 | 55.544 | 71.266 | 33.302 | 1.00 | 76.76 | 7 |
| 10 | ATOM | 6343 | C | GLN | D | 178 | 61.219 | 73.240 | 33.936 | 1.00 | 71.25 | 6 |
| | ATOM | 6344 | O | GLN | D | 178 | 61.226 | 74.368 | 33.462 | 1.00 | 71.24 | 8 |
| | ATOM | 6345 | N | LYS | D | 179 | 62.291 | 72.461 | 33.979 | 1.00 | 71.70 | 7 |
| | ATOM | 6346 | CA | LYS | D | 179 | 63.593 | 72.904 | 33.474 | 1.00 | 71.59 | 6 |
| | ATOM | 6347 | CB | LYS | D | 179 | 64.553 | 73.170 | 34.642 | 1.00 | 73.63 | 6 |
| 15 | ATOM | 6348 | CG | LYS | D | 179 | 63.906 | 73.953 | 35.800 | 1.00 | 77.80 | 6 |
| | ATOM | 6349 | CD | LYS | D | 179 | 64.795 | 74.018 | 37.040 | 1.00 | 78.53 | 6 |
| | ATOM | 6350 | CE | LYS | D | 179 | 64.016 | 74.470 | 38.273 | 1.00 | 79.16 | 6 |
| | ATOM | 6351 | NZ | LYS | D | 179 | 62.899 | 73.537 | 38.610 | 1.00 | 77.90 | 7 |
| | ATOM | 6352 | C | LYS | D | 179 | 64.173 | 71.807 | 32.601 | 1.00 | 70.50 | 6 |
| 20 | ATOM | 6353 | O | LYS | D | 179 | 64.549 | 70.754 | 33.112 | 1.00 | 69.32 | 8 |
| | ATOM | 6354 | N | LYS | D | 180 | 64.252 | 72.044 | 31.294 | 1.00 | 69.56 | 7 |
| | ATOM | 6355 | CA | LYS | D | 180 | 64.803 | 71.039 | 30.382 | 1.00 | 69.55 | 6 |
| | ATOM | 6356 | CB | LYS | D | 180 | 64.581 | 71.464 | 28.924 | 1.00 | 69.05 | 6 |
| | ATOM | 6357 | CG | LYS | D | 180 | 65.462 | 72.584 | 28.419 | 1.00 | 68.35 | 6 |
| 25 | ATOM | 6358 | CD | LYS | D | 180 | 66.773 | 72.041 | 27.860 | 1.00 | 66.86 | 6 |
| | ATOM | 6359 | CE | LYS | D | 180 | 66.550 | 71.200 | 26.619 | 1.00 | 63.97 | 6 |
| | ATOM | 6360 | NZ | LYS | D | 180 | 66.096 | 72.020 | 25.476 | 1.00 | 64.54 | 7 |
| | ATOM | 6361 | C | LYS | D | 180 | 66.293 | 70.795 | 30.642 | 1.00 | 68.87 | 6 |
| | ATOM | 6362 | O | LYS | D | 180 | 66.869 | 71.406 | 31.536 | 1.00 | 69.83 | 8 |
| 30 | ATOM | 6363 | N | ASN | D | 181 | 66.905 | 69.879 | 29.897 | 1.00 | 68.37 | 7 |
| | ATOM | 6364 | CA | ASN | D | 181 | 68.326 | 69.615 | 30.060 | 1.00 | 70.05 | 6 |
| | ATOM | 6365 | CB | ASN | D | 181 | 68.711 | 69.461 | 31.540 | 1.00 | 70.86 | 6 |
| | ATOM | 6366 | CG | ASN | D | 181 | 67.808 | 68.533 | 32.291 | 1.00 | 71.68 | 6 |
| | ATOM | 6367 | OD1 | ASN | D | 181 | 67.498 | 67.446 | 31.823 | 1.00 | 74.38 | 8 |
| 35 | ATOM | 6368 | ND2 | ASN | D | 181 | 67.395 | 68.945 | 33.487 | 1.00 | 72.61 | 7 |
| | ATOM | 6369 | C | ASN | D | 181 | 68.905 | 68.449 | 29.281 | 1.00 | 70.12 | 6 |
| | ATOM | 6370 | O | ASN | D | 181 | 68.535 | 67.303 | 29.491 | 1.00 | 68.91 | 8 |
| | ATOM | 6371 | N | SER | D | 182 | 69.844 | 68.760 | 28.385 | 1.00 | 71.81 | 7 |
| | ATOM | 6372 | CA | SER | D | 182 | 70.519 | 67.744 | 27.577 | 1.00 | 71.83 | 6 |
| 40 | ATOM | 6373 | CB | SER | D | 182 | 71.361 | 68.418 | 26.495 | 1.00 | 70.60 | 6 |
| | ATOM | 6374 | OG | SER | D | 182 | 71.817 | 67.463 | 25.557 | 1.00 | 71.86 | 8 |
| | ATOM | 6375 | C | SER | D | 182 | 71.405 | 66.866 | 28.482 | 1.00 | 71.03 | 6 |
| | ATOM | 6376 | O | SER | D | 182 | 71.794 | 67.281 | 29.572 | 1.00 | 72.13 | 8 |
| | ATOM | 6377 | N | VAL | D | 183 | 71.715 | 65.653 | 28.037 | 1.00 | 70.45 | 7 |
| 45 | ATOM | 6378 | CA | VAL | D | 183 | 72.528 | 64.736 | 28.842 | 1.00 | 69.61 | 6 |
| | ATOM | 6379 | CB | VAL | D | 183 | 71.728 | 64.221 | 30.066 | 1.00 | 69.93 | 6 |
| | ATOM | 6380 | CG1 | VAL | D | 183 | 70.268 | 63.988 | 29.671 | 1.00 | 71.71 | 6 |
| | ATOM | 6381 | CG2 | VAL | D | 183 | 72.331 | 62.909 | 30.584 | 1.00 | 68.31 | 6 |
| | ATOM | 6382 | C | VAL | D | 183 | 73.046 | 63.521 | 28.069 | 1.00 | 69.82 | 6 |
| 50 | ATOM | 6383 | O | VAL | D | 183 | 72.317 | 62.887 | 27.305 | 1.00 | 69.28 | 8 |
| | ATOM | 6384 | N | THR | D | 184 | 74.314 | 63.194 | 28.272 | 1.00 | 71.03 | 7 |
| | ATOM | 6385 | CA | THR | D | 184 | 74.898 | 62.041 | 27.596 | 1.00 | 72.40 | 6 |
| | ATOM | 6386 | CB | THR | D | 184 | 76.314 | 62.360 | 27.027 | 1.00 | 71.67 | 6 |
| | ATOM | 6387 | OG1 | THR | D | 184 | 76.207 | 63.364 | 26.010 | 1.00 | 69.65 | 8 |
| 55 | ATOM | 6388 | CG2 | THR | D | 184 | 76.944 | 61.110 | 26.404 | 1.00 | 71.24 | 6 |
| | ATOM | 6389 | C | THR | D | 184 | 74.997 | 60.901 | 28.602 | 1.00 | 73.76 | 6 |
| | ATOM | 6390 | O | THR | D | 184 | 75.273 | 61.132 | 29.786 | 1.00 | 74.26 | 8 |
| | ATOM | 6391 | N | TYR | D | 185 | 74.749 | 59.679 | 28.139 | 1.00 | 74.82 | 7 |
| | ATOM | 6392 | CA | TYR | D | 185 | 74.818 | 58.515 | 29.024 | 1.00 | 76.20 | 6 |
| 60 | ATOM | 6393 | CB | TYR | D | 185 | 73.477 | 57.755 | 29.046 | 1.00 | 77.17 | 6 |
| | ATOM | 6394 | CG | TYR | D | 185 | 72.286 | 58.637 | 29.324 | 1.00 | 77.03 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 6395 | CD1 | TYR | D | 185 | 71.822 | 59.527 | 28.362 | 1.00 | 77.16 | 6 |
| | ATOM | 6396 | CE1 | TYR | D | 185 | 70.781 | 60.416 | 28.640 | 1.00 | 78.65 | 6 |
| | ATOM | 6397 | CD2 | TYR | D | 185 | 71.676 | 58.643 | 30.578 | 1.00 | 78.44 | 6 |
| | ATOM | 6398 | CE2 | TYR | D | 185 | 70.629 | 59.532 | 30.873 | 1.00 | 78.76 | 6 |
| 5 | ATOM | 6399 | CZ | TYR | D | 185 | 70.190 | 60.417 | 29.897 | 1.00 | 78.44 | 6 |
| | ATOM | 6400 | OH | TYR | D | 185 | 69.173 | 61.311 | 30.160 | 1.00 | 78.64 | 8 |
| | ATOM | 6401 | C | TYR | D | 185 | 75.909 | 57.595 | 28.525 | 1.00 | 76.37 | 6 |
| | ATOM | 6402 | O | TYR | D | 185 | 76.062 | 57.403 | 27.320 | 1.00 | 75.86 | 8 |
| 10 | ATOM | 6403 | N | SER | D | 186 | 76.669 | 57.031 | 29.454 | 1.00 | 78.41 | 7 |
| | ATOM | 6404 | CA | SER | D | 186 | 77.762 | 56.127 | 29.097 | 1.00 | 80.47 | 6 |
| | ATOM | 6405 | CB | SER | D | 186 | 78.353 | 55.494 | 30.361 | 1.00 | 80.37 | 6 |
| | ATOM | 6406 | OG | SER | D | 186 | 77.324 | 55.000 | 31.202 | 1.00 | 80.82 | 8 |
| | ATOM | 6407 | C | SER | D | 186 | 77.259 | 55.042 | 28.139 | 1.00 | 81.49 | 6 |
| | ATOM | 6408 | O | SER | D | 186 | 77.977 | 54.637 | 27.205 | 1.00 | 80.86 | 8 |
| 15 | ATOM | 6409 | N | CYS | D | 187 | 76.018 | 54.601 | 28.370 | 1.00 | 82.03 | 7 |
| | ATOM | 6410 | CA | CYS | D | 187 | 75.366 | 53.573 | 27.553 | 1.00 | 82.11 | 6 |
| | ATOM | 6411 | C | CYS | D | 187 | 75.259 | 54.005 | 26.123 | 1.00 | 82.74 | 6 |
| | ATOM | 6412 | O | CYS | D | 187 | 75.445 | 53.226 | 25.179 | 1.00 | 81.67 | 8 |
| 20 | ATOM | 6413 | CB | CYS | D | 187 | 73.908 | 53.360 | 27.980 | 1.00 | 82.28 | 6 |
| | ATOM | 6414 | SG | CYS | D | 187 | 72.725 | 54.778 | 27.707 | 1.00 | 81.64 | 16 |
| | ATOM | 6415 | N | CYS | D | 188 | 74.954 | 55.287 | 25.990 | 1.00 | 83.43 | 7 |
| | ATOM | 6416 | CA | CYS | D | 188 | 74.614 | 55.827 | 24.701 | 1.00 | 83.03 | 6 |
| | ATOM | 6417 | C | CYS | D | 188 | 75.379 | 57.070 | 24.204 | 1.00 | 81.94 | 6 |
| 25 | ATOM | 6418 | O | CYS | D | 188 | 75.401 | 58.127 | 24.860 | 1.00 | 81.77 | 8 |
| | ATOM | 6419 | CB | CYS | D | 188 | 73.091 | 56.059 | 24.777 | 1.00 | 83.56 | 6 |
| | ATOM | 6420 | SG | CYS | D | 188 | 72.115 | 54.783 | 25.740 | 1.00 | 85.15 | 16 |
| | ATOM | 6421 | N | PRO | D | 189 | 76.000 | 56.945 | 23.013 | 1.00 | 80.60 | 7 |
| | ATOM | 6422 | CD | PRO | D | 189 | 75.862 | 55.676 | 22.263 | 1.00 | 80.05 | 6 |
| 30 | ATOM | 6423 | CA | PRO | D | 189 | 76.809 | 57.921 | 22.254 | 1.00 | 78.99 | 6 |
| | ATOM | 6424 | CB | PRO | D | 189 | 76.804 | 57.341 | 20.836 | 1.00 | 79.15 | 6 |
| | ATOM | 6425 | CG | PRO | D | 189 | 76.835 | 55.852 | 21.097 | 1.00 | 80.06 | 6 |
| | ATOM | 6426 | C | PRO | D | 189 | 76.386 | 59.408 | 22.258 | 1.00 | 76.71 | 6 |
| | ATOM | 6427 | O | PRO | D | 189 | 77.106 | 60.265 | 22.777 | 1.00 | 76.06 | 8 |
| 35 | ATOM | 6428 | N | GLU | D | 190 | 75.237 | 59.713 | 21.663 | 1.00 | 73.54 | 7 |
| | ATOM | 6429 | CA | GLU | D | 190 | 74.762 | 61.101 | 21.583 | 1.00 | 70.67 | 6 |
| | ATOM | 6430 | CB | GLU | D | 190 | 73.735 | 61.233 | 20.462 | 1.00 | 72.95 | 6 |
| | ATOM | 6431 | CG | GLU | D | 190 | 73.941 | 60.272 | 19.292 | 1.00 | 76.22 | 6 |
| | ATOM | 6432 | CD | GLU | D | 190 | 74.959 | 60.778 | 18.284 | 1.00 | 77.17 | 6 |
| 40 | ATOM | 6433 | OE1 | GLU | D | 190 | 74.920 | 61.987 | 17.949 | 1.00 | 75.78 | 8 |
| | ATOM | 6434 | OE2 | GLU | D | 190 | 75.786 | 59.961 | 17.819 | 1.00 | 78.06 | 8 |
| | ATOM | 6435 | C | GLU | D | 190 | 74.113 | 61.576 | 22.874 | 1.00 | 67.13 | 6 |
| | ATOM | 6436 | O | GLU | D | 190 | 74.060 | 60.842 | 23.861 | 1.00 | 66.77 | 8 |
| | ATOM | 6437 | N | ALA | D | 191 | 73.595 | 62.797 | 22.852 | 1.00 | 63.73 | 7 |
| 45 | ATOM | 6438 | CA | ALA | D | 191 | 72.924 | 63.362 | 24.027 | 1.00 | 63.96 | 6 |
| | ATOM | 6439 | CB | ALA | D | 191 | 73.293 | 64.833 | 24.188 | 1.00 | 60.91 | 6 |
| | ATOM | 6440 | C | ALA | D | 191 | 71.398 | 63.226 | 23.935 | 1.00 | 63.09 | 6 |
| | ATOM | 6441 | O | ALA | D | 191 | 70.824 | 63.324 | 22.848 | 1.00 | 63.27 | 8 |
| | ATOM | 6442 | N | TYR | D | 192 | 70.737 | 63.015 | 25.073 | 1.00 | 61.86 | 7 |
| 50 | ATOM | 6443 | CA | TYR | D | 192 | 69.284 | 62.883 | 25.077 | 1.00 | 60.02 | 6 |
| | ATOM | 6444 | CB | TYR | D | 192 | 68.874 | 61.483 | 25.544 | 1.00 | 58.87 | 6 |
| | ATOM | 6445 | CG | TYR | D | 192 | 69.185 | 60.408 | 24.531 | 1.00 | 59.77 | 6 |
| | ATOM | 6446 | CD1 | TYR | D | 192 | 70.447 | 59.804 | 24.491 | 1.00 | 59.82 | 6 |
| | ATOM | 6447 | CE1 | TYR | D | 192 | 70.762 | 58.849 | 23.514 | 1.00 | 59.91 | 6 |
| 55 | ATOM | 6448 | CD2 | TYR | D | 192 | 68.234 | 60.030 | 23.568 | 1.00 | 59.23 | 6 |
| | ATOM | 6449 | CE2 | TYR | D | 192 | 68.534 | 59.084 | 22.592 | 1.00 | 60.37 | 6 |
| | ATOM | 6450 | CZ | TYR | D | 192 | 69.803 | 58.496 | 22.566 | 1.00 | 61.99 | 6 |
| | ATOM | 6451 | OH | TYR | D | 192 | 70.120 | 57.582 | 21.581 | 1.00 | 61.54 | 8 |
| | ATOM | 6452 | C | TYR | D | 192 | 68.590 | 63.938 | 25.922 | 1.00 | 59.37 | 6 |
| 60 | ATOM | 6453 | O | TYR | D | 192 | 68.594 | 63.874 | 27.150 | 1.00 | 61.63 | 8 |
| | ATOM | 6454 | N | GLU | D | 193 | 67.986 | 64.909 | 25.248 | 1.00 | 59.03 | 7 |
| | ATOM | 6455 | CA | GLU | D | 193 | 67.280 | 65.992 | 25.915 | 1.00 | 60.46 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 6456 | CB | GLU D 193 | 66.832 | 67.054 | 24.898 | 1.00 | 61.02 | 6 |
| | ATOM | 6457 | CG | GLU D 193 | 67.985 | 67.781 | 24.196 | 1.00 | 65.53 | 6 |
| | ATOM | 6458 | CD | GLU D 193 | 67.522 | 68.937 | 23.292 | 1.00 | 66.58 | 6 |
| | ATOM | 6459 | OE1 | GLU D 193 | 66.678 | 69.760 | 23.739 | 1.00 | 66.15 | 8 |
| | ATOM | 6460 | OE2 | GLU D 193 | 68.017 | 69.023 | 22.138 | 1.00 | 66.88 | 8 |
| 10 | ATOM | 6461 | C | GLU D 193 | 66.066 | 65.455 | 26.658 | 1.00 | 61.32 | 6 |
| | ATOM | 6462 | O | GLU D 193 | 65.498 | 64.428 | 26.278 | 1.00 | 61.10 | 8 |
| | ATOM | 6463 | N | ASP D 194 | 65.682 | 66.157 | 27.724 | 1.00 | 62.11 | 7 |
| | ATOM | 6464 | CA | ASP D 194 | 64.533 | 65.788 | 28.537 | 1.00 | 60.32 | 6 |
| | ATOM | 6465 | CB | ASP D 194 | 64.855 | 64.571 | 29.416 | 1.00 | 60.68 | 6 |
| 15 | ATOM | 6466 | CG | ASP D 194 | 65.759 | 64.907 | 30.589 | 1.00 | 61.25 | 6 |
| | ATOM | 6467 | OD1 | ASP D 194 | 66.929 | 64.453 | 30.591 | 1.00 | 62.58 | 8 |
| | ATOM | 6468 | OD2 | ASP D 194 | 65.297 | 65.619 | 31.509 | 1.00 | 61.10 | 8 |
| | ATOM | 6469 | C | ASP D 194 | 64.086 | 66.951 | 29.417 | 1.00 | 59.85 | 6 |
| | ATOM | 6470 | O | ASP D 194 | 64.890 | 67.793 | 29.816 | 1.00 | 60.03 | 8 |
| 20 | ATOM | 6471 | N | VAL D 195 | 62.792 | 66.993 | 29.704 | 1.00 | 57.38 | 7 |
| | ATOM | 6472 | CA | VAL D 195 | 62.225 | 68.024 | 30.538 | 1.00 | 55.36 | 6 |
| | ATOM | 6473 | CB | VAL D 195 | 60.864 | 68.480 | 30.001 | 1.00 | 52.24 | 6 |
| | ATOM | 6474 | CG1 | VAL D 195 | 60.179 | 69.394 | 31.001 | 1.00 | 51.69 | 6 |
| | ATOM | 6475 | CG2 | VAL D 195 | 61.058 | 69.189 | 28.693 | 1.00 | 52.14 | 6 |
| 25 | ATOM | 6476 | C | VAL D 195 | 62.044 | 67.460 | 31.935 | 1.00 | 56.36 | 6 |
| | ATOM | 6477 | O | VAL D 195 | 61.452 | 66.412 | 32.114 | 1.00 | 57.76 | 8 |
| | ATOM | 6478 | N | GLU D 196 | 62.571 | 68.151 | 32.930 | 1.00 | 58.67 | 7 |
| | ATOM | 6479 | CA | GLU D 196 | 62.425 | 67.712 | 34.303 | 1.00 | 58.26 | 6 |
| | ATOM | 6480 | CB | GLU D 196 | 63.754 | 67.833 | 35.035 | 1.00 | 58.61 | 6 |
| 30 | ATOM | 6481 | CG | GLU D 196 | 63.725 | 67.326 | 36.460 | 1.00 | 61.95 | 6 |
| | ATOM | 6482 | CD | GLU D 196 | 65.062 | 67.533 | 37.172 | 1.00 | 63.50 | 6 |
| | ATOM | 6483 | OE1 | GLU D 196 | 66.083 | 67.014 | 36.679 | 1.00 | 62.21 | 8 |
| | ATOM | 6484 | OE2 | GLU D 196 | 65.099 | 68.218 | 38.222 | 1.00 | 65.74 | 8 |
| | ATOM | 6485 | C | GLU D 196 | 61.370 | 68.598 | 34.959 | 1.00 | 58.08 | 6 |
| 35 | ATOM | 6486 | O | GLU D 196 | 61.500 | 69.822 | 34.997 | 1.00 | 59.87 | 8 |
| | ATOM | 6487 | N | VAL D 197 | 60.305 | 67.979 | 35.452 | 1.00 | 57.22 | 7 |
| | ATOM | 6488 | CA | VAL D 197 | 59.242 | 68.721 | 36.104 | 1.00 | 54.36 | 6 |
| | ATOM | 6489 | CB | VAL D 197 | 57.863 | 68.304 | 35.567 | 1.00 | 52.68 | 6 |
| | ATOM | 6490 | CG1 | VAL D 197 | 56.772 | 69.095 | 36.255 | 1.00 | 49.60 | 6 |
| 40 | ATOM | 6491 | CG2 | VAL D 197 | 57.809 | 68.517 | 34.068 | 1.00 | 50.84 | 6 |
| | ATOM | 6492 | C | VAL D 197 | 59.317 | 68.420 | 37.587 | 1.00 | 55.10 | 6 |
| | ATOM | 6493 | O | VAL D 197 | 59.367 | 67.264 | 37.995 | 1.00 | 55.27 | 8 |
| | ATOM | 6494 | N | SER D 198 | 59.351 | 69.467 | 38.399 | 1.00 | 56.68 | 7 |
| | ATOM | 6495 | CA | SER D 198 | 59.413 | 69.284 | 39.839 | 1.00 | 56.39 | 6 |
| 45 | ATOM | 6496 | CB | SER D 198 | 60.487 | 70.188 | 40.448 | 1.00 | 55.89 | 6 |
| | ATOM | 6497 | OG | SER D 198 | 61.789 | 69.767 | 40.066 | 1.00 | 57.83 | 8 |
| | ATOM | 6498 | C | SER D 198 | 58.058 | 69.593 | 40.448 | 1.00 | 56.61 | 6 |
| | ATOM | 6499 | O | SER D 198 | 57.536 | 70.698 | 40.317 | 1.00 | 56.25 | 8 |
| | ATOM | 6500 | N | LEU D 199 | 57.481 | 68.597 | 41.101 | 1.00 | 56.92 | 7 |
| 50 | ATOM | 6501 | CA | LEU D 199 | 56.189 | 68.770 | 41.728 | 1.00 | 56.84 | 6 |
| | ATOM | 6502 | CB | LEU D 199 | 55.303 | 67.561 | 41.468 | 1.00 | 57.08 | 6 |
| | ATOM | 6503 | CG | LEU D 199 | 53.981 | 67.553 | 42.243 | 1.00 | 57.99 | 6 |
| | ATOM | 6504 | CD1 | LEU D 199 | 53.094 | 68.726 | 41.834 | 1.00 | 57.12 | 6 |
| | ATOM | 6505 | CD2 | LEU D 199 | 53.272 | 66.246 | 41.971 | 1.00 | 58.22 | 6 |
| 55 | ATOM | 6506 | C | LEU D 199 | 56.354 | 68.953 | 43.220 | 1.00 | 57.85 | 6 |
| | ATOM | 6507 | O | LEU D 199 | 56.625 | 67.998 | 43.950 | 1.00 | 58.46 | 8 |
| | ATOM | 6508 | N | ASN D 200 | 56.207 | 70.192 | 43.671 | 1.00 | 58.52 | 7 |
| | ATOM | 6509 | CA | ASN D 200 | 56.315 | 70.486 | 45.084 | 1.00 | 57.07 | 6 |
| | ATOM | 6510 | CB | ASN D 200 | 57.017 | 71.827 | 45.311 | 1.00 | 59.47 | 6 |
| 60 | ATOM | 6511 | CG | ASN D 200 | 57.126 | 72.184 | 46.781 | 1.00 | 61.26 | 6 |
| | ATOM | 6512 | OD1 | ASN D 200 | 57.508 | 71.359 | 47.613 | 1.00 | 60.78 | 8 |
| | ATOM | 6513 | ND2 | ASN D 200 | 56.792 | 73.423 | 47.108 | 1.00 | 63.13 | 7 |
| | ATOM | 6514 | C | ASN D 200 | 54.886 | 70.533 | 45.593 | 1.00 | 55.28 | 6 |
| | ATOM | 6515 | O | ASN D 200 | 54.108 | 71.422 | 45.242 | 1.00 | 53.93 | 8 |
| | ATOM | 6516 | N | PHE D 201 | 54.549 | 69.554 | 46.419 | 1.00 | 53.26 | 7 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 6517 | CA | PHE | D | 201 | 53.218 | 69.444 | 46.973 | 1.00 | 51.91 | 6 |
| | ATOM | 6518 | CB | PHE | D | 201 | 52.408 | 68.434 | 46.168 | 1.00 | 49.89 | 6 |
| | ATOM | 6519 | CG | PHE | D | 201 | 52.870 | 67.013 | 46.348 | 1.00 | 46.59 | 6 |
| 5 | ATOM | 6520 | CD1 | PHE | D | 201 | 52.068 | 66.086 | 47.003 | 1.00 | 45.61 | 6 |
| | ATOM | 6521 | CD2 | PHE | D | 201 | 54.133 | 66.613 | 45.903 | 1.00 | 46.86 | 6 |
| | ATOM | 6522 | CE1 | PHE | D | 201 | 52.519 | 64.779 | 47.218 | 1.00 | 45.68 | 6 |
| | ATOM | 6523 | CE2 | PHE | D | 201 | 54.597 | 65.312 | 46.112 | 1.00 | 44.48 | 6 |
| | ATOM | 6524 | CZ | PHE | D | 201 | 53.788 | 64.394 | 46.772 | 1.00 | 44.43 | 6 |
| 10 | ATOM | 6525 | C | PHE | D | 201 | 53.360 | 68.940 | 48.386 | 1.00 | 53.35 | 6 |
| | ATOM | 6526 | O | PHE | D | 201 | 54.456 | 68.570 | 48.818 | 1.00 | 52.18 | 8 |
| | ATOM | 6527 | N | ARG | D | 202 | 52.238 | 68.902 | 49.093 | 1.00 | 55.22 | 7 |
| | ATOM | 6528 | CA | ARG | D | 202 | 52.211 | 68.426 | 50.470 | 1.00 | 57.74 | 6 |
| | ATOM | 6529 | CB | ARG | D | 202 | 52.632 | 69.546 | 51.412 | 1.00 | 58.53 | 6 |
| | ATOM | 6530 | CG | ARG | D | 202 | 51.564 | 70.612 | 51.484 | 1.00 | 62.76 | 6 |
| 15 | ATOM | 6531 | CD | ARG | D | 202 | 51.956 | 71.797 | 52.313 | 1.00 | 64.76 | 6 |
| | ATOM | 6532 | NE | ARG | D | 202 | 50.901 | 72.806 | 52.296 | 1.00 | 64.52 | 7 |
| | ATOM | 6533 | CZ | ARG | D | 202 | 51.046 | 74.035 | 52.779 | 1.00 | 65.00 | 6 |
| | ATOM | 6534 | NH1 | ARG | D | 202 | 52.206 | 74.409 | 53.323 | 1.00 | 65.86 | 7 |
| | ATOM | 6535 | NH2 | ARG | D | 202 | 50.045 | 74.896 | 52.708 | 1.00 | 62.46 | 7 |
| 20 | ATOM | 6536 | C | ARG | D | 202 | 50.788 | 67.997 | 50.835 | 1.00 | 57.64 | 6 |
| | ATOM | 6537 | O | ARG | D | 202 | 49.822 | 68.392 | 50.186 | 1.00 | 55.63 | 8 |
| | ATOM | 6538 | N | LYS | D | 203 | 50.668 | 67.189 | 51.878 | 1.00 | 58.55 | 7 |
| | ATOM | 6539 | CA | LYS | D | 203 | 49.359 | 66.759 | 52.332 | 1.00 | 59.55 | 6 |
| | ATOM | 6540 | CB | LYS | D | 203 | 49.505 | 65.708 | 53.428 | 1.00 | 60.97 | 6 |
| 25 | ATOM | 6541 | CG | LYS | D | 203 | 48.195 | 65.258 | 54.031 | 1.00 | 62.61 | 6 |
| | ATOM | 6542 | CD | LYS | D | 203 | 48.445 | 64.319 | 55.194 | 1.00 | 66.11 | 6 |
| | ATOM | 6543 | CE | LYS | D | 203 | 47.142 | 63.813 | 55.784 | 1.00 | 68.33 | 6 |
| | ATOM | 6544 | NZ | LYS | D | 203 | 46.380 | 62.985 | 54.804 | 1.00 | 69.98 | 7 |
| | ATOM | 6545 | C | LYS | D | 203 | 48.702 | 68.008 | 52.914 | 1.00 | 60.27 | 6 |
| 30 | ATOM | 6546 | O | LYS | D | 203 | 49.402 | 68.886 | 53.428 | 1.00 | 60.55 | 8 |
| | ATOM | 6547 | N | LYS | D | 204 | 47.374 | 68.105 | 52.832 | 1.00 | 59.32 | 7 |
| | ATOM | 6548 | CA | LYS | D | 204 | 46.680 | 69.260 | 53.395 | 1.00 | 60.40 | 6 |
| | ATOM | 6549 | CB | LYS | D | 204 | 45.221 | 69.284 | 52.947 | 1.00 | 59.66 | 6 |
| | ATOM | 6550 | CG | LYS | D | 204 | 45.054 | 69.738 | 51.495 | 1.00 | 56.15 | 6 |
| 35 | ATOM | 6551 | CD | LYS | D | 204 | 43.652 | 69.489 | 50.974 | 1.00 | 52.10 | 6 |
| | ATOM | 6552 | CE | LYS | D | 204 | 43.593 | 69.775 | 49.488 | 1.00 | 52.88 | 6 |
| | ATOM | 6553 | NZ | LYS | D | 204 | 42.334 | 69.320 | 48.856 | 1.00 | 54.65 | 7 |
| | ATOM | 6554 | C | LYS | D | 204 | 46.776 | 69.201 | 54.919 | 1.00 | 62.27 | 6 |
| | ATOM | 6555 | O | LYS | D | 204 | 47.031 | 68.129 | 55.479 | 1.00 | 63.85 | 8 |
| 40 | ATOM | 6556 | N | GLY | D | 205 | 46.590 | 70.344 | 55.587 | 1.00 | 61.70 | 7 |
| | ATOM | 6557 | CA | GLY | D | 205 | 46.701 | 70.390 | 57.043 | 1.00 | 61.46 | 6 |
| | ATOM | 6558 | C | GLY | D | 205 | 45.432 | 70.704 | 57.821 | 1.00 | 60.96 | 6 |
| | ATOM | 6559 | OT1 | GLY | D | 205 | 44.364 | 70.809 | 57.191 | 1.00 | 61.45 | 8 |
| | ATOM | 6560 | OT2 | GLY | D | 205 | 45.495 | 70.835 | 59.067 | 1.00 | 60.53 | 8 |
| 45 | ATOM | 6561 | CB | PHE | E | 1 | 68.481 | 57.493 | 1.362 | 1.00 | 63.85 | 6 |
| | ATOM | 6562 | CG | PHE | E | 1 | 68.496 | 56.384 | 0.357 | 1.00 | 65.93 | 6 |
| | ATOM | 6563 | CD1 | PHE | E | 1 | 67.431 | 56.207 | -0.526 | 1.00 | 67.13 | 6 |
| | ATOM | 6564 | CD2 | PHE | E | 1 | 69.549 | 55.462 | 0.345 | 1.00 | 67.48 | 6 |
| | ATOM | 6565 | CE1 | PHE | E | 1 | 67.410 | 55.116 | -1.409 | 1.00 | 68.65 | 6 |
| 50 | ATOM | 6566 | CE2 | PHE | E | 1 | 69.548 | 54.364 | -0.528 | 1.00 | 67.48 | 6 |
| | ATOM | 6567 | CZ | PHE | E | 1 | 68.481 | 54.185 | -1.406 | 1.00 | 69.10 | 6 |
| | ATOM | 6568 | C | PHE | E | 1 | 67.191 | 59.419 | 2.218 | 1.00 | 61.93 | 6 |
| | ATOM | 6569 | O | PHE | E | 1 | 67.898 | 59.384 | 3.225 | 1.00 | 62.32 | 8 |
| | ATOM | 6570 | N | PHE | E | 1 | 68.457 | 59.591 | 0.037 | 1.00 | 62.93 | 7 |
| 55 | ATOM | 6571 | CA | PHE | E | 1 | 67.655 | 58.712 | 0.943 | 1.00 | 62.89 | 6 |
| | ATOM | 6572 | N | ASP | E | 2 | 66.011 | 60.038 | 2.205 | 1.00 | 61.01 | 7 |
| | ATOM | 6573 | CA | ASP | E | 2 | 65.524 | 60.730 | 3.406 | 1.00 | 60.82 | 6 |
| | ATOM | 6574 | CB | ASP | E | 2 | 64.448 | 61.754 | 3.027 | 1.00 | 59.66 | 6 |
| | ATOM | 6575 | CG | ASP | E | 2 | 63.263 | 61.126 | 2.346 | 1.00 | 61.52 | 6 |
| 60 | ATOM | 6576 | OD1 | ASP | E | 2 | 62.587 | 60.347 | 3.035 | 1.00 | 62.72 | 8 |
| | ATOM | 6577 | OD2 | ASP | E | 2 | 63.006 | 61.396 | 1.142 | 1.00 | 60.96 | 8 |

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|----|------|------|-----|-----|---|------|--------|--------|--------|--------------|
| 5 | ATOM | 6578 | C | ASP | E | 2 | 65.012 | 59.731 | 4.459 | 1.00 60.89 6 |
| | ATOM | 6579 | O | ASP | E | 2 | 64.990 | 58.525 | 4.216 | 1.00 62.95 8 |
| | ATOM | 6580 | N | ARG | E | 3 | 64.624 | 60.214 | 5.635 | 1.00 60.20 7 |
| | ATOM | 6581 | CA | ARG | E | 3 | 64.161 | 59.321 | 6.697 | 1.00 57.08 6 |
| | ATOM | 6582 | CB | ARG | E | 3 | 63.746 | 60.128 | 7.933 | 1.00 56.21 6 |
| 10 | ATOM | 6583 | CG | ARG | E | 3 | 64.906 | 60.475 | 8.878 | 1.00 56.67 6 |
| | ATOM | 6584 | CD | ARG | E | 3 | 65.314 | 59.266 | 9.702 | 1.00 57.53 6 |
| | ATOM | 6585 | NE | ARG | E | 3 | 66.519 | 59.426 | 10.524 | 1.00 58.61 7 |
| | ATOM | 6586 | CZ | ARG | E | 3 | 66.825 | 60.497 | 11.258 | 1.00 60.79 6 |
| | ATOM | 6587 | NH1 | ARG | E | 3 | 66.024 | 61.559 | 11.294 | 1.00 61.35 7 |
| 15 | ATOM | 6588 | NH2 | ARG | E | 3 | 67.943 | 60.499 | 11.975 | 1.00 58.97 7 |
| | ATOM | 6589 | C | ARG | E | 3 | 63.008 | 58.447 | 6.244 | 1.00 56.93 6 |
| | ATOM | 6590 | O | ARG | E | 3 | 62.949 | 57.256 | 6.567 | 1.00 58.08 8 |
| | ATOM | 6591 | N | ALA | E | 4 | 62.102 | 59.033 | 5.473 | 1.00 54.21 7 |
| | ATOM | 6592 | CA | ALA | E | 4 | 60.937 | 58.311 | 4.993 | 1.00 52.85 6 |
| 20 | ATOM | 6593 | CB | ALA | E | 4 | 60.002 | 59.262 | 4.270 | 1.00 50.53 6 |
| | ATOM | 6594 | C | ALA | E | 4 | 61.342 | 57.168 | 4.075 | 1.00 53.00 6 |
| | ATOM | 6595 | O | ALA | E | 4 | 60.858 | 56.056 | 4.225 | 1.00 53.30 8 |
| | ATOM | 6596 | N | ASP | E | 5 | 62.235 | 57.443 | 3.132 | 1.00 54.00 7 |
| | ATOM | 6597 | CA | ASP | E | 5 | 62.692 | 56.433 | 2.190 | 1.00 54.02 6 |
| 25 | ATOM | 6598 | CB | ASP | E | 5 | 63.702 | 57.021 | 1.197 | 1.00 56.37 6 |
| | ATOM | 6599 | CG | ASP | E | 5 | 63.153 | 58.223 | 0.435 | 1.00 60.25 6 |
| | ATOM | 6600 | OD1 | ASP | E | 5 | 62.018 | 58.154 | -0.072 | 1.00 61.70 8 |
| | ATOM | 6601 | OD2 | ASP | E | 5 | 63.864 | 59.247 | 0.327 | 1.00 64.63 8 |
| | ATOM | 6602 | C | ASP | E | 5 | 63.341 | 55.278 | 2.924 | 1.00 54.45 6 |
| 30 | ATOM | 6603 | O | ASP | E | 5 | 63.192 | 54.127 | 2.532 | 1.00 54.26 8 |
| | ATOM | 6604 | N | ILE | E | 6 | 64.060 | 55.582 | 3.997 | 1.00 54.54 7 |
| | ATOM | 6605 | CA | ILE | E | 6 | 64.734 | 54.535 | 4.755 | 1.00 55.28 6 |
| | ATOM | 6606 | CB | ILE | E | 6 | 65.727 | 55.121 | 5.781 | 1.00 56.90 6 |
| | ATOM | 6607 | CG2 | ILE | E | 6 | 66.476 | 53.991 | 6.489 | 1.00 56.40 6 |
| 35 | ATOM | 6608 | CG1 | ILE | E | 6 | 66.728 | 56.031 | 5.068 | 1.00 58.74 6 |
| | ATOM | 6609 | CD1 | ILE | E | 6 | 67.833 | 56.589 | 5.976 | 1.00 60.73 6 |
| | ATOM | 6610 | C | ILE | E | 6 | 63.765 | 53.617 | 5.482 | 1.00 53.47 6 |
| | ATOM | 6611 | O | ILE | E | 6 | 63.830 | 52.401 | 5.322 | 1.00 53.23 8 |
| | ATOM | 6612 | N | LEU | E | 7 | 62.883 | 54.199 | 6.290 | 1.00 53.23 7 |
| 40 | ATOM | 6613 | CA | LEU | E | 7 | 61.897 | 53.423 | 7.033 | 1.00 52.57 6 |
| | ATOM | 6614 | CB | LEU | E | 7 | 61.060 | 54.354 | 7.899 | 1.00 52.03 6 |
| | ATOM | 6615 | CG | LEU | E | 7 | 61.862 | 55.020 | 9.017 | 1.00 52.39 6 |
| | ATOM | 6616 | CD1 | LEU | E | 7 | 61.074 | 56.183 | 9.607 | 1.00 53.72 6 |
| | ATOM | 6617 | CD2 | LEU | E | 7 | 62.185 | 53.989 | 10.070 | 1.00 47.50 6 |
| 45 | ATOM | 6618 | C | LEU | E | 7 | 61.003 | 52.660 | 6.065 | 1.00 52.40 6 |
| | ATOM | 6619 | O | LEU | E | 7 | 60.665 | 51.503 | 6.302 | 1.00 53.43 8 |
| | ATOM | 6620 | N | TYR | E | 8 | 60.644 | 53.311 | 4.967 | 1.00 51.20 7 |
| | ATOM | 6621 | CA | TYR | E | 8 | 59.810 | 52.707 | 3.951 | 1.00 52.74 6 |
| | ATOM | 6622 | CB | TYR | E | 8 | 59.622 | 53.686 | 2.804 | 1.00 54.75 6 |
| 50 | ATOM | 6623 | CG | TYR | E | 8 | 58.825 | 53.102 | 1.660 | 1.00 60.00 6 |
| | ATOM | 6624 | CD1 | TYR | E | 8 | 57.448 | 52.902 | 1.773 | 1.00 59.81 6 |
| | ATOM | 6625 | CE1 | TYR | E | 8 | 56.723 | 52.341 | 0.734 | 1.00 59.72 6 |
| | ATOM | 6626 | CD2 | TYR | E | 8 | 59.453 | 52.717 | 0.465 | 1.00 61.59 6 |
| | ATOM | 6627 | CE2 | TYR | E | 8 | 58.727 | 52.148 | -0.580 | 1.00 59.67 6 |
| 55 | ATOM | 6628 | CZ | TYR | E | 8 | 57.367 | 51.967 | -0.433 | 1.00 59.94 6 |
| | ATOM | 6629 | OH | TYR | E | 8 | 56.646 | 51.411 | -1.457 | 1.00 63.44 8 |
| | ATOM | 6630 | C | TYR | E | 8 | 60.399 | 51.405 | 3.404 | 1.00 54.02 6 |
| | ATOM | 6631 | O | TYR | E | 8 | 59.692 | 50.414 | 3.259 | 1.00 54.84 8 |
| | ATOM | 6632 | N | ASN | E | 9 | 61.688 | 51.411 | 3.082 | 1.00 53.58 7 |
| 60 | ATOM | 6633 | CA | ASN | E | 9 | 62.338 | 50.224 | 2.559 | 1.00 52.96 6 |
| | ATOM | 6634 | CB | ASN | E | 9 | 63.790 | 50.524 | 2.182 | 1.00 58.69 6 |
| | ATOM | 6635 | CG | ASN | E | 9 | 63.907 | 51.445 | 0.966 | 1.00 62.10 6 |
| | ATOM | 6636 | OD1 | ASN | E | 9 | 62.908 | 51.771 | 0.321 | 1.00 64.59 8 |
| | ATOM | 6637 | ND2 | ASN | E | 9 | 65.137 | 51.861 | 0.645 | 1.00 63.43 7 |
| | ATOM | 6638 | C | ASN | E | 9 | 62.297 | 49.112 | 3.584 | 1.00 52.17 6 |

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|----|------|------|-----|-----|---|------|--------|--------|--------|--------------|
| 5 | ATOM | 6639 | O | ASN | E | 9 | 61.870 | 48.003 | 3.287 | 1.00 51.04 8 |
| | ATOM | 6640 | N | ILE | E | 10 | 62.746 | 49.410 | 4.794 | 1.00 53.05 7 |
| | ATOM | 6641 | CA | ILE | E | 10 | 62.752 | 48.424 | 5.866 | 1.00 53.91 6 |
| | ATOM | 6642 | CB | ILE | E | 10 | 63.189 | 49.053 | 7.195 | 1.00 53.67 6 |
| | ATOM | 6643 | CG2 | ILE | E | 10 | 63.060 | 48.027 | 8.316 | 1.00 51.86 6 |
| 10 | ATOM | 6644 | CG1 | ILE | E | 10 | 64.627 | 49.564 | 7.077 | 1.00 51.89 6 |
| | ATOM | 6645 | CD1 | ILE | E | 10 | 65.085 | 50.379 | 8.251 | 1.00 50.06 6 |
| | ATOM | 6646 | C | ILE | E | 10 | 61.358 | 47.835 | 6.054 | 1.00 55.10 6 |
| | ATOM | 6647 | O | ILE | E | 10 | 61.186 | 46.631 | 6.216 | 1.00 55.00 8 |
| | ATOM | 6648 | N | ARG | E | 11 | 60.364 | 48.708 | 6.032 | 1.00 56.28 7 |
| 15 | ATOM | 6649 | CA | ARG | E | 11 | 58.975 | 48.308 | 6.199 | 1.00 57.92 6 |
| | ATOM | 6650 | CB | ARG | E | 11 | 58.084 | 49.543 | 6.106 | 1.00 61.96 6 |
| | ATOM | 6651 | CG | ARG | E | 11 | 56.628 | 49.280 | 6.323 | 1.00 69.38 6 |
| | ATOM | 6652 | CD | ARG | E | 11 | 56.359 | 49.040 | 7.797 | 1.00 79.46 6 |
| | ATOM | 6653 | NE | ARG | E | 11 | 54.957 | 49.274 | 8.149 | 1.00 85.84 7 |
| 20 | ATOM | 6654 | CZ | ARG | E | 11 | 54.244 | 50.315 | 7.713 | 1.00 89.11 6 |
| | ATOM | 6655 | NH1 | ARG | E | 11 | 54.801 | 51.215 | 6.892 | 1.00 90.35 7 |
| | ATOM | 6656 | NH2 | ARG | E | 11 | 52.980 | 50.475 | 8.117 | 1.00 90.14 7 |
| | ATOM | 6657 | C | ARG | E | 11 | 58.559 | 47.314 | 5.126 | 1.00 56.77 6 |
| | ATOM | 6658 | O | ARG | E | 11 | 57.986 | 46.264 | 5.415 | 1.00 55.32 8 |
| 25 | ATOM | 6659 | N | GLN | E | 12 | 58.866 | 47.663 | 3.881 | 1.00 56.51 7 |
| | ATOM | 6660 | CA | GLN | E | 12 | 58.511 | 46.850 | 2.730 | 1.00 54.24 6 |
| | ATOM | 6661 | CB | GLN | E | 12 | 58.583 | 47.698 | 1.485 | 1.00 53.75 6 |
| | ATOM | 6662 | CG | GLN | E | 12 | 57.341 | 47.645 | 0.673 | 1.00 58.35 6 |
| | ATOM | 6663 | CD | GLN | E | 12 | 56.287 | 48.540 | 1.223 | 1.00 59.21 6 |
| 30 | ATOM | 6664 | OE1 | GLN | E | 12 | 56.517 | 49.726 | 1.375 | 1.00 63.59 8 |
| | ATOM | 6665 | NE2 | GLN | E | 12 | 55.121 | 47.990 | 1.528 | 1.00 59.83 7 |
| | ATOM | 6666 | C | GLN | E | 12 | 59.312 | 45.581 | 2.484 | 1.00 53.65 6 |
| | ATOM | 6667 | O | GLN | E | 12 | 58.820 | 44.677 | 1.825 | 1.00 52.67 8 |
| | ATOM | 6668 | N | THR | E | 13 | 60.536 | 45.507 | 2.995 | 1.00 54.14 7 |
| 35 | ATOM | 6669 | CA | THR | E | 13 | 61.369 | 44.331 | 2.771 | 1.00 55.96 6 |
| | ATOM | 6670 | CB | THR | E | 13 | 62.714 | 44.726 | 2.181 | 1.00 55.93 6 |
| | ATOM | 6671 | OG1 | THR | E | 13 | 63.380 | 45.612 | 3.090 | 1.00 55.29 8 |
| | ATOM | 6672 | CG2 | THR | E | 13 | 62.526 | 45.400 | 0.822 | 1.00 55.33 6 |
| | ATOM | 6673 | C | THR | E | 13 | 61.656 | 43.486 | 4.005 | 1.00 58.24 6 |
| 40 | ATOM | 6674 | O | THR | E | 13 | 62.096 | 42.343 | 3.892 | 1.00 58.85 8 |
| | ATOM | 6675 | N | SER | E | 14 | 61.414 | 44.042 | 5.182 | 1.00 60.49 7 |
| | ATOM | 6676 | CA | SER | E | 14 | 61.681 | 43.317 | 6.408 | 1.00 61.17 6 |
| | ATOM | 6677 | CB | SER | E | 14 | 61.629 | 44.265 | 7.599 | 1.00 62.69 6 |
| | ATOM | 6678 | OG | SER | E | 14 | 62.247 | 43.658 | 8.723 | 1.00 66.18 8 |
| 45 | ATOM | 6679 | C | SER | E | 14 | 60.727 | 42.151 | 6.644 | 1.00 60.36 6 |
| | ATOM | 6680 | O | SER | E | 14 | 59.579 | 42.153 | 6.184 | 1.00 59.94 8 |
| | ATOM | 6681 | N | ARG | E | 15 | 61.233 | 41.156 | 7.369 | 1.00 58.70 7 |
| | ATOM | 6682 | CA | ARG | E | 15 | 60.487 | 39.949 | 7.703 | 1.00 58.01 6 |
| | ATOM | 6683 | CB | ARG | E | 15 | 60.926 | 38.792 | 6.805 | 1.00 57.94 6 |
| 50 | ATOM | 6684 | CG | ARG | E | 15 | 60.686 | 39.058 | 5.325 | 1.00 59.93 6 |
| | ATOM | 6685 | CD | ARG | E | 15 | 60.746 | 37.761 | 4.547 | 1.00 63.77 6 |
| | ATOM | 6686 | NE | ARG | E | 15 | 59.755 | 36.818 | 5.060 | 1.00 66.81 7 |
| | ATOM | 6687 | CZ | ARG | E | 15 | 59.714 | 35.516 | 4.772 | 1.00 66.79 6 |
| | ATOM | 6688 | NH1 | ARG | E | 15 | 60.622 | 34.982 | 3.964 | 1.00 64.79 7 |
| 55 | ATOM | 6689 | NH2 | ARG | E | 15 | 58.748 | 34.752 | 5.287 | 1.00 67.36 7 |
| | ATOM | 6690 | C | ARG | E | 15 | 60.743 | 39.621 | 9.170 | 1.00 55.75 6 |
| | ATOM | 6691 | O | ARG | E | 15 | 61.705 | 38.928 | 9.513 | 1.00 55.70 8 |
| | ATOM | 6692 | N | PRO | E | 16 | 59.869 | 40.121 | 10.057 | 1.00 54.09 7 |
| | ATOM | 6693 | CD | PRO | E | 16 | 58.682 | 40.932 | 9.727 | 1.00 50.97 6 |
| 60 | ATOM | 6694 | CA | PRO | E | 16 | 59.961 | 39.919 | 11.503 | 1.00 51.94 6 |
| | ATOM | 6695 | CB | PRO | E | 16 | 58.731 | 40.650 | 12.031 | 1.00 50.89 6 |
| | ATOM | 6696 | CG | PRO | E | 16 | 58.463 | 41.680 | 10.997 | 1.00 51.98 6 |
| | ATOM | 6697 | C | PRO | E | 16 | 59.986 | 38.473 | 11.945 | 1.00 50.22 6 |
| | ATOM | 6698 | O | PRO | E | 16 | 60.418 | 38.176 | 13.046 | 1.00 49.19 8 |
| | ATOM | 6699 | N | ASP | E | 17 | 59.512 | 37.579 | 11.095 | 1.00 50.78 7 |

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| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 6700 | CA | ASP | E | 17 | 59.477 | 36.171 | 11.446 | 1.00 | 53.11 | 6 |
| | ATOM | 6701 | CB | ASP | E | 17 | 58.244 | 35.492 | 10.832 | 1.00 | 58.78 | 6 |
| | ATOM | 6702 | CG | ASP | E | 17 | 56.931 | 35.917 | 11.513 | 1.00 | 64.95 | 6 |
| | ATOM | 6703 | OD1 | ASP | E | 17 | 56.959 | 36.261 | 12.732 | 1.00 | 65.29 | 8 |
| 5 | ATOM | 6704 | OD2 | ASP | E | 17 | 55.865 | 35.887 | 10.831 | 1.00 | 66.80 | 8 |
| | ATOM | 6705 | C | ASP | E | 17 | 60.716 | 35.401 | 11.039 | 1.00 | 52.04 | 6 |
| | ATOM | 6706 | O | ASP | E | 17 | 60.787 | 34.194 | 11.242 | 1.00 | 53.16 | 8 |
| | ATOM | 6707 | N | VAL | E | 18 | 61.701 | 36.090 | 10.481 | 1.00 | 52.13 | 7 |
| | ATOM | 6708 | CA | VAL | E | 18 | 62.906 | 35.410 | 10.034 | 1.00 | 51.75 | 6 |
| 10 | ATOM | 6709 | CB | VAL | E | 18 | 63.050 | 35.519 | 8.509 | 1.00 | 53.20 | 6 |
| | ATOM | 6710 | CG1 | VAL | E | 18 | 64.265 | 34.728 | 8.037 | 1.00 | 54.22 | 6 |
| | ATOM | 6711 | CG2 | VAL | E | 18 | 61.797 | 35.010 | 7.843 | 1.00 | 52.93 | 6 |
| | ATOM | 6712 | C | VAL | E | 18 | 64.193 | 35.897 | 10.675 | 1.00 | 50.84 | 6 |
| | ATOM | 6713 | O | VAL | E | 18 | 64.595 | 37.039 | 10.513 | 1.00 | 50.74 | 8 |
| 15 | ATOM | 6714 | N | ILE | E | 19 | 64.841 | 34.990 | 11.387 | 1.00 | 51.04 | 7 |
| | ATOM | 6715 | CA | ILE | E | 19 | 66.092 | 35.270 | 12.077 | 1.00 | 53.80 | 6 |
| | ATOM | 6716 | CB | ILE | E | 19 | 66.478 | 34.027 | 12.940 | 1.00 | 52.99 | 6 |
| | ATOM | 6717 | CG2 | ILE | E | 19 | 66.791 | 32.842 | 12.040 | 1.00 | 52.72 | 6 |
| | ATOM | 6718 | CG1 | ILE | E | 19 | 67.644 | 34.346 | 13.870 | 1.00 | 52.81 | 6 |
| 20 | ATOM | 6719 | CD1 | ILE | E | 19 | 67.867 | 33.290 | 14.923 | 1.00 | 49.41 | 6 |
| | ATOM | 6720 | C | ILE | E | 19 | 67.184 | 35.628 | 11.053 | 1.00 | 55.50 | 6 |
| | ATOM | 6721 | O | ILE | E | 19 | 67.399 | 34.903 | 10.087 | 1.00 | 54.87 | 8 |
| | ATOM | 6722 | N | PRO | E | 20 | 67.879 | 36.765 | 11.250 | 1.00 | 57.80 | 7 |
| | ATOM | 6723 | CD | PRO | E | 20 | 67.710 | 37.684 | 12.385 | 1.00 | 58.20 | 6 |
| 25 | ATOM | 6724 | CA | PRO | E | 20 | 68.948 | 37.253 | 10.359 | 1.00 | 60.68 | 6 |
| | ATOM | 6725 | CB | PRO | E | 20 | 69.252 | 38.664 | 10.897 | 1.00 | 58.99 | 6 |
| | ATOM | 6726 | CG | PRO | E | 20 | 68.056 | 39.007 | 11.744 | 1.00 | 60.19 | 6 |
| | ATOM | 6727 | C | PRO | E | 20 | 70.201 | 36.370 | 10.360 | 1.00 | 62.73 | 6 |
| | ATOM | 6728 | O | PRO | E | 20 | 71.317 | 36.854 | 10.568 | 1.00 | 61.22 | 8 |
| 30 | ATOM | 6729 | N | THR | E | 21 | 70.008 | 35.080 | 10.117 | 1.00 | 65.32 | 7 |
| | ATOM | 6730 | CA | THR | E | 21 | 71.107 | 34.128 | 10.106 | 1.00 | 69.19 | 6 |
| | ATOM | 6731 | CB | THR | E | 21 | 70.573 | 32.698 | 10.364 | 1.00 | 68.56 | 6 |
| | ATOM | 6732 | OG1 | THR | E | 21 | 70.744 | 32.370 | 11.751 | 1.00 | 66.59 | 8 |
| | ATOM | 6733 | CG2 | THR | E | 21 | 71.300 | 31.677 | 9.502 | 1.00 | 68.21 | 6 |
| 35 | ATOM | 6734 | C | THR | E | 21 | 71.964 | 34.121 | 8.840 | 1.00 | 72.78 | 6 |
| | ATOM | 6735 | O | THR | E | 21 | 71.450 | 34.096 | 7.716 | 1.00 | 72.75 | 8 |
| | ATOM | 6736 | N | GLN | E | 22 | 73.282 | 34.128 | 9.051 | 1.00 | 77.19 | 7 |
| | ATOM | 6737 | CA | GLN | E | 22 | 74.279 | 34.102 | 7.971 | 1.00 | 80.45 | 6 |
| | ATOM | 6738 | CB | GLN | E | 22 | 75.303 | 35.209 | 8.192 | 1.00 | 81.20 | 6 |
| 40 | ATOM | 6739 | CG | GLN | E | 22 | 74.691 | 36.597 | 8.264 | 1.00 | 83.07 | 6 |
| | ATOM | 6740 | CD | GLN | E | 22 | 75.515 | 37.542 | 9.131 | 1.00 | 85.11 | 6 |
| | ATOM | 6741 | OE1 | GLN | E | 22 | 75.640 | 37.329 | 10.355 | 1.00 | 85.67 | 8 |
| | ATOM | 6742 | NE2 | GLN | E | 22 | 76.087 | 38.587 | 8.510 | 1.00 | 84.48 | 7 |
| | ATOM | 6743 | C | GLN | E | 22 | 74.980 | 32.739 | 8.023 | 1.00 | 81.85 | 6 |
| 45 | ATOM | 6744 | O | GLN | E | 22 | 75.783 | 32.480 | 8.929 | 1.00 | 81.74 | 8 |
| | ATOM | 6745 | N | ARG | E | 23 | 74.676 | 31.880 | 7.050 | 1.00 | 84.04 | 7 |
| | ATOM | 6746 | CA | ARG | E | 23 | 75.235 | 30.521 | 7.001 | 1.00 | 84.92 | 6 |
| | ATOM | 6747 | CB | ARG | E | 23 | 76.767 | 30.550 | 6.931 | 1.00 | 84.82 | 6 |
| | ATOM | 6748 | CG | ARG | E | 23 | 77.314 | 30.929 | 5.558 | 1.00 | 87.29 | 6 |
| 50 | ATOM | 6749 | CD | ARG | E | 23 | 77.788 | 32.397 | 5.462 | 1.00 | 90.43 | 6 |
| | ATOM | 6750 | NE | ARG | E | 23 | 78.140 | 32.777 | 4.081 | 1.00 | 92.74 | 7 |
| | ATOM | 6751 | CZ | ARG | E | 23 | 78.982 | 32.103 | 3.287 | 1.00 | 93.28 | 6 |
| | ATOM | 6752 | NH1 | ARG | E | 23 | 79.592 | 30.993 | 3.712 | 1.00 | 92.22 | 7 |
| | ATOM | 6753 | NH2 | ARG | E | 23 | 79.204 | 32.535 | 2.047 | 1.00 | 92.78 | 7 |
| 55 | ATOM | 6754 | C | ARG | E | 23 | 74.790 | 29.736 | 8.237 | 1.00 | 85.32 | 6 |
| | ATOM | 6755 | O | ARG | E | 23 | 73.673 | 29.929 | 8.747 | 1.00 | 85.55 | 8 |
| | ATOM | 6756 | N | ASP | E | 24 | 75.648 | 28.842 | 8.718 | 1.00 | 85.95 | 7 |
| | ATOM | 6757 | CA | ASP | E | 24 | 75.304 | 28.062 | 9.907 | 1.00 | 86.37 | 6 |
| | ATOM | 6758 | CB | ASP | E | 24 | 76.103 | 26.752 | 9.985 | 1.00 | 90.45 | 6 |
| 60 | ATOM | 6759 | CG | ASP | E | 24 | 76.671 | 26.317 | 8.636 | 1.00 | 93.77 | 6 |
| | ATOM | 6760 | OD1 | ASP | E | 24 | 75.856 | 26.082 | 7.698 | 1.00 | 95.19 | 8 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 6761 | OD2 | ASP | E | 24 | 77.930 | 26.212 | 8.533 | 1.00 | 94.96 | 8 | |
| | ATOM | 6762 | C | ASP | E | 24 | 75.657 | 28.917 | 11.116 | 1.00 | 84.76 | 6 | |
| | ATOM | 6763 | O | ASP | E | 24 | 75.551 | 28.466 | 12.259 | 1.00 | 84.92 | 8 | |
| | ATOM | 6764 | N | ARG | E | 25 | 76.097 | 30.146 | 10.857 | 1.00 | 82.51 | 7 | |
| | ATOM | 6765 | CA | ARG | E | 25 | 76.465 | 31.063 | 11.930 | 1.00 | 80.45 | 6 | |
| | ATOM | 6766 | CB | ARG | E | 25 | 77.208 | 32.289 | 11.382 | 1.00 | 83.04 | 6 | |
| | ATOM | 6767 | CG | ARG | E | 25 | 78.635 | 32.032 | 10.918 | 1.00 | 87.73 | 6 | |
| | ATOM | 6768 | CD | ARG | E | 25 | 79.370 | 33.358 | 10.688 | 1.00 | 91.97 | 6 | |
| 10 | ATOM | 6769 | NE | ARG | E | 25 | 80.781 | 33.171 | 10.340 | 1.00 | 95.94 | 7 | |
| | ATOM | 6770 | CZ | ARG | E | 25 | 81.667 | 34.164 | 10.199 | 1.00 | 97.73 | 6 | |
| | ATOM | 6771 | NH1 | ARG | E | 25 | 81.285 | 35.435 | 10.379 | 1.00 | 98.12 | 7 | |
| | ATOM | 6772 | NH2 | ARG | E | 25 | 82.938 | 33.892 | 9.880 | 1.00 | 97.12 | 7 | |
| 15 | ATOM | 6773 | C | ARG | E | 25 | 75.256 | 31.557 | 12.708 | 1.00 | 76.54 | 6 | |
| | ATOM | 6774 | O | ARG | E | 25 | 74.265 | 31.999 | 12.122 | 1.00 | 76.16 | 8 | |
| | ATOM | 6775 | N | PRO | E | 26 | 75.322 | 31.483 | 14.045 | 1.00 | 73.86 | 7 | |
| | ATOM | 6776 | CD | PRO | E | 26 | 76.343 | 30.778 | 14.834 | 1.00 | 73.05 | 6 | |
| | ATOM | 6777 | CA | PRO | E | 26 | 74.231 | 31.936 | 14.916 | 1.00 | 70.73 | 6 | |
| | ATOM | 6778 | CB | PRO | E | 26 | 74.647 | 31.425 | 16.295 | 1.00 | 70.99 | 6 | |
| | ATOM | 6779 | CG | PRO | E | 26 | 75.529 | 30.257 | 15.984 | 1.00 | 72.42 | 6 | |
| | ATOM | 6780 | C | PRO | E | 26 | 74.199 | 33.466 | 14.891 | 1.00 | 67.63 | 6 | |
| 20 | ATOM | 6781 | O | PRO | E | 26 | 75.173 | 34.110 | 14.493 | 1.00 | 66.91 | 8 | |
| | ATOM | 6782 | N | VAL | E | 27 | 73.076 | 34.046 | 15.288 | 1.00 | 63.36 | 7 | |
| | ATOM | 6783 | CA | VAL | E | 27 | 72.980 | 35.487 | 15.346 | 1.00 | 57.94 | 6 | |
| | ATOM | 6784 | CB | VAL | E | 27 | 71.537 | 35.949 | 15.266 | 1.00 | 55.79 | 6 | |
| | ATOM | 6785 | CG1 | VAL | E | 27 | 71.403 | 37.366 | 15.780 | 1.00 | 54.61 | 6 | |
| | ATOM | 6786 | CG2 | VAL | E | 27 | 71.082 | 35.870 | 13.839 | 1.00 | 57.04 | 6 | |
| | ATOM | 6787 | C | VAL | E | 27 | 73.554 | 35.821 | 16.706 | 1.00 | 57.83 | 6 | |
| | ATOM | 6788 | O | VAL | E | 27 | 73.180 | 35.207 | 17.711 | 1.00 | 58.05 | 8 | |
| 30 | ATOM | 6789 | N | ALA | E | 28 | 74.490 | 36.760 | 16.744 | 1.00 | 55.79 | 7 | |
| | ATOM | 6790 | CA | ALA | E | 28 | 75.087 | 37.130 | 18.014 | 1.00 | 55.59 | 6 | |
| | ATOM | 6791 | CB | ALA | E | 28 | 76.508 | 37.588 | 17.810 | 1.00 | 54.25 | 6 | |
| | ATOM | 6792 | C | ALA | E | 28 | 74.270 | 38.224 | 18.677 | 1.00 | 54.76 | 6 | |
| | ATOM | 6793 | O | ALA | E | 28 | 74.244 | 39.370 | 18.216 | 1.00 | 54.28 | 8 | |
| | ATOM | 6794 | N | VAL | E | 29 | 73.596 | 37.850 | 19.759 | 1.00 | 53.10 | 7 | |
| | ATOM | 6795 | CA | VAL | E | 29 | 72.769 | 38.783 | 20.514 | 1.00 | 53.62 | 6 | |
| | ATOM | 6796 | CB | VAL | E | 29 | 71.338 | 38.222 | 20.767 | 1.00 | 52.63 | 6 | |
| 35 | ATOM | 6797 | CG1 | VAL | E | 29 | 70.531 | 39.210 | 21.591 | 1.00 | 47.51 | 6 | |
| | ATOM | 6798 | CG2 | VAL | E | 29 | 70.641 | 37.940 | 19.446 | 1.00 | 52.51 | 6 | |
| | ATOM | 6799 | C | VAL | E | 29 | 73.412 | 39.051 | 21.865 | 1.00 | 53.21 | 6 | |
| | ATOM | 6800 | O | VAL | E | 29 | 73.760 | 38.119 | 22.599 | 1.00 | 53.58 | 8 | |
| | ATOM | 6801 | N | SER | E | 30 | 73.583 | 40.325 | 22.184 | 1.00 | 51.51 | 7 | |
| | ATOM | 6802 | CA | SER | E | 30 | 74.154 | 40.681 | 23.459 | 1.00 | 54.05 | 6 | |
| | ATOM | 6803 | CB | SER | E | 30 | 75.288 | 41.690 | 23.276 | 1.00 | 52.43 | 6 | |
| | ATOM | 6804 | OG | SER | E | 30 | 74.821 | 42.854 | 22.632 | 1.00 | 55.74 | 8 | |
| 45 | ATOM | 6805 | C | SER | E | 30 | 73.024 | 41.277 | 24.301 | 1.00 | 56.57 | 6 | |
| | ATOM | 6806 | O | SER | E | 30 | 72.236 | 42.110 | 23.825 | 1.00 | 54.93 | 8 | |
| | ATOM | 6807 | N | VAL | E | 31 | 72.946 | 40.824 | 25.550 | 1.00 | 58.33 | 7 | |
| | ATOM | 6808 | CA | VAL | E | 31 | 71.934 | 41.280 | 26.493 | 1.00 | 60.16 | 6 | |
| | ATOM | 6809 | CB | VAL | E | 31 | 71.058 | 40.118 | 26.966 | 1.00 | 59.85 | 6 | |
| | ATOM | 6810 | CG1 | VAL | E | 31 | 69.842 | 40.662 | 27.700 | 1.00 | 60.72 | 6 | |
| | ATOM | 6811 | CG2 | VAL | E | 31 | 70.653 | 39.264 | 25.783 | 1.00 | 60.11 | 6 | |
| | ATOM | 6812 | C | VAL | E | 31 | 72.599 | 41.891 | 27.724 | 1.00 | 61.00 | 6 | |
| 50 | ATOM | 6813 | O | VAL | E | 31 | 73.542 | 41.327 | 28.279 | 1.00 | 62.05 | 8 | |
| | ATOM | 6814 | N | SER | E | 32 | 72.092 | 43.037 | 28.160 | 1.00 | 61.21 | 7 | |
| | ATOM | 6815 | CA | SER | E | 32 | 72.648 | 43.717 | 29.318 | 1.00 | 60.47 | 6 | |
| | ATOM | 6816 | CB | SER | E | 32 | 73.688 | 44.743 | 28.851 | 1.00 | 61.09 | 6 | |
| | ATOM | 6817 | OG | SER | E | 32 | 74.162 | 45.553 | 29.919 | 1.00 | 63.13 | 8 | |
| | ATOM | 6818 | C | SER | E | 32 | 71.552 | 44.422 | 30.111 | 1.00 | 60.62 | 6 | |
| | ATOM | 6819 | O | SER | E | 32 | 70.941 | 45.375 | 29.621 | 1.00 | 62.55 | 8 | |
| | ATOM | 6820 | N | LEU | E | 33 | 71.300 | 43.962 | 31.332 | 1.00 | 58.26 | 7 | |
| 60 | ATOM | 6821 | CA | LEU | E | 33 | 70.282 | 44.591 | 32.165 | 1.00 | 56.62 | 6 | |

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|----|------|------|-----|----------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 6822 | CB | LEU E 33 | 69.658 | 43.578 | 33.122 | 1.00 | 54.43 | 6 | |
| | ATOM | 6823 | CG | LEU E 33 | 69.031 | 42.344 | 32.487 | 1.00 | 55.79 | 6 | |
| | ATOM | 6824 | CD1 | LEU E 33 | 68.247 | 41.561 | 33.532 | 1.00 | 53.82 | 6 | |
| | ATOM | 6825 | CD2 | LEU E 33 | 68.132 | 42.781 | 31.348 | 1.00 | 56.32 | 6 | |
| | ATOM | 6826 | C | LEU E 33 | 70.880 | 45.717 | 32.985 | 1.00 | 56.68 | 6 | |
| 10 | ATOM | 6827 | O | LEU E 33 | 71.954 | 45.572 | 33.556 | 1.00 | 58.07 | 8 | |
| | ATOM | 6828 | N | LYS E 34 | 70.186 | 46.843 | 33.029 | 1.00 | 55.71 | 7 | |
| | ATOM | 6829 | CA | LYS E 34 | 70.616 | 47.978 | 33.822 | 1.00 | 54.48 | 6 | |
| | ATOM | 6830 | CB | LYS E 34 | 70.799 | 49.207 | 32.948 | 1.00 | 57.11 | 6 | |
| | ATOM | 6831 | CG | LYS E 34 | 71.726 | 48.985 | 31.774 | 1.00 | 66.06 | 6 | |
| 15 | ATOM | 6832 | CD | LYS E 34 | 73.179 | 48.679 | 32.205 | 1.00 | 71.51 | 6 | |
| | ATOM | 6833 | CE | LYS E 34 | 74.103 | 48.409 | 30.973 | 1.00 | 73.37 | 6 | |
| | ATOM | 6834 | NZ | LYS E 34 | 75.541 | 48.135 | 31.351 | 1.00 | 72.80 | 7 | |
| | ATOM | 6835 | C | LYS E 34 | 69.459 | 48.201 | 34.776 | 1.00 | 53.15 | 6 | |
| | ATOM | 6836 | O | LYS E 34 | 68.373 | 48.590 | 34.356 | 1.00 | 52.81 | 8 | |
| 20 | ATOM | 6837 | N | PHE E 35 | 69.668 | 47.947 | 36.059 | 1.00 | 51.67 | 7 | |
| | ATOM | 6838 | CA | PHE E 35 | 68.584 | 48.120 | 37.011 | 1.00 | 49.05 | 6 | |
| | ATOM | 6839 | CB | PHE E 35 | 68.890 | 47.364 | 38.292 | 1.00 | 46.62 | 6 | |
| | ATOM | 6840 | CG | PHE E 35 | 68.921 | 45.883 | 38.095 | 1.00 | 47.20 | 6 | |
| | ATOM | 6841 | CD1 | PHE E 35 | 70.071 | 45.254 | 37.651 | 1.00 | 46.38 | 6 | |
| 25 | ATOM | 6842 | CD2 | PHE E 35 | 67.766 | 45.125 | 38.253 | 1.00 | 49.08 | 6 | |
| | ATOM | 6843 | CE1 | PHE E 35 | 70.074 | 43.897 | 37.363 | 1.00 | 47.59 | 6 | |
| | ATOM | 6844 | CE2 | PHE E 35 | 67.755 | 43.760 | 37.964 | 1.00 | 48.98 | 6 | |
| | ATOM | 6845 | CZ | PHE E 35 | 68.913 | 43.145 | 37.517 | 1.00 | 48.13 | 6 | |
| | ATOM | 6846 | C | PHE E 35 | 68.225 | 49.560 | 37.285 | 1.00 | 48.83 | 6 | |
| 30 | ATOM | 6847 | O | PHE E 35 | 69.086 | 50.401 | 37.492 | 1.00 | 50.99 | 8 | |
| | ATOM | 6848 | N | ILE E 36 | 66.927 | 49.831 | 37.259 | 1.00 | 47.58 | 7 | |
| | ATOM | 6849 | CA | ILE E 36 | 66.403 | 51.166 | 37.465 | 1.00 | 44.93 | 6 | |
| | ATOM | 6850 | CB | ILE E 36 | 65.398 | 51.532 | 36.370 | 1.00 | 44.37 | 6 | |
| | ATOM | 6851 | CG2 | ILE E 36 | 64.927 | 52.956 | 36.547 | 1.00 | 39.93 | 6 | |
| 35 | ATOM | 6852 | CG1 | ILE E 36 | 66.034 | 51.328 | 34.994 | 1.00 | 45.24 | 6 | |
| | ATOM | 6853 | CD1 | ILE E 36 | 67.290 | 52.114 | 34.776 | 1.00 | 46.74 | 6 | |
| | ATOM | 6854 | C | ILE E 36 | 65.698 | 51.266 | 38.792 | 1.00 | 46.03 | 6 | |
| | ATOM | 6855 | O | ILE E 36 | 65.588 | 52.350 | 39.347 | 1.00 | 46.58 | 8 | |
| | ATOM | 6856 | N | ASN E 37 | 65.201 | 50.142 | 39.299 | 1.00 | 45.38 | 7 | |
| 40 | ATOM | 6857 | CA | ASN E 37 | 64.510 | 50.163 | 40.580 | 1.00 | 44.10 | 6 | |
| | ATOM | 6858 | CB | ASN E 37 | 63.256 | 51.022 | 40.471 | 1.00 | 42.99 | 6 | |
| | ATOM | 6859 | CG | ASN E 37 | 62.870 | 51.660 | 41.784 | 1.00 | 46.14 | 6 | |
| | ATOM | 6860 | OD1 | ASN E 37 | 62.892 | 51.018 | 42.832 | 1.00 | 45.55 | 8 | |
| | ATOM | 6861 | ND2 | ASN E 37 | 62.497 | 52.931 | 41.731 | 1.00 | 45.29 | 7 | |
| 45 | ATOM | 6862 | C | ASN E 37 | 64.125 | 48.777 | 41.087 | 1.00 | 45.25 | 6 | |
| | ATOM | 6863 | O | ASN E 37 | 64.009 | 47.825 | 40.317 | 1.00 | 42.90 | 8 | |
| | ATOM | 6864 | N | ILE E 38 | 63.951 | 48.680 | 42.401 | 1.00 | 46.26 | 7 | |
| | ATOM | 6865 | CA | ILE E 38 | 63.537 | 47.453 | 43.057 | 1.00 | 47.22 | 6 | |
| | ATOM | 6866 | CB | ILE E 38 | 64.646 | 46.913 | 43.940 | 1.00 | 46.57 | 6 | |
| 50 | ATOM | 6867 | CG2 | ILE E 38 | 64.152 | 45.692 | 44.685 | 1.00 | 46.43 | 6 | |
| | ATOM | 6868 | CG1 | ILE E 38 | 65.848 | 46.561 | 43.058 | 1.00 | 47.22 | 6 | |
| | ATOM | 6869 | CD1 | ILE E 38 | 67.109 | 46.207 | 43.784 | 1.00 | 46.51 | 6 | |
| | ATOM | 6870 | C | ILE E 38 | 62.346 | 47.902 | 43.879 | 1.00 | 48.14 | 6 | |
| | ATOM | 6871 | O | ILE E 38 | 62.504 | 48.619 | 44.855 | 1.00 | 49.04 | 8 | |
| 55 | ATOM | 6872 | N | LEU E 39 | 61.157 | 47.476 | 43.466 | 1.00 | 49.65 | 7 | |
| | ATOM | 6873 | CA | LEU E 39 | 59.908 | 47.897 | 44.092 | 1.00 | 51.44 | 6 | |
| | ATOM | 6874 | CB | LEU E 39 | 58.856 | 48.052 | 43.004 | 1.00 | 53.02 | 6 | |
| | ATOM | 6875 | CG | LEU E 39 | 59.359 | 48.916 | 41.847 | 1.00 | 54.99 | 6 | |
| | ATOM | 6876 | CD1 | LEU E 39 | 58.314 | 49.019 | 40.767 | 1.00 | 54.07 | 6 | |
| 60 | ATOM | 6877 | CD2 | LEU E 39 | 59.717 | 50.289 | 42.377 | 1.00 | 53.65 | 6 | |
| | ATOM | 6878 | C | LEU E 39 | 59.312 | 47.104 | 45.241 | 1.00 | 52.90 | 6 | |
| | ATOM | 6879 | O | LEU E 39 | 58.795 | 47.690 | 46.184 | 1.00 | 53.53 | 8 | |
| | ATOM | 6880 | N | GLU E 40 | 59.332 | 45.781 | 45.163 | 1.00 | 54.20 | 7 | |
| | ATOM | 6881 | CA | GLU E 40 | 58.781 | 44.988 | 46.249 | 1.00 | 56.14 | 6 | |
| | ATOM | 6882 | CB | GLU E 40 | 57.357 | 44.549 | 45.960 | 1.00 | 58.59 | 6 | |

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|----|------|------|-----|-----|------|--------|--------|--------|------|---------|
| 5 | ATOM | 6883 | CG | GLU | E 40 | 56.377 | 45.678 | 45.865 | 1.00 | 64.95 6 |
| | ATOM | 6884 | CD | GLU | E 40 | 54.960 | 45.178 | 45.718 | 1.00 | 68.54 6 |
| | ATOM | 6885 | OE1 | GLU | E 40 | 54.697 | 44.405 | 44.757 | 1.00 | 70.88 8 |
| | ATOM | 6886 | OE2 | GLU | E 40 | 54.119 | 45.561 | 46.564 | 1.00 | 69.89 8 |
| | ATOM | 6887 | C | GLU | E 40 | 59.620 | 43.773 | 46.449 | 1.00 | 55.88 6 |
| 10 | ATOM | 6888 | O | GLU | E 40 | 60.029 | 43.134 | 45.498 | 1.00 | 58.42 8 |
| | ATOM | 6889 | N | VAL | E 41 | 59.876 | 43.454 | 47.700 | 1.00 | 55.75 7 |
| | ATOM | 6890 | CA | VAL | E 41 | 60.675 | 42.300 | 48.021 | 1.00 | 55.46 6 |
| | ATOM | 6891 | CB | VAL | E 41 | 62.067 | 42.732 | 48.550 | 1.00 | 56.94 6 |
| | ATOM | 6892 | CG1 | VAL | E 41 | 62.802 | 41.547 | 49.107 | 1.00 | 58.11 6 |
| 15 | ATOM | 6893 | CG2 | VAL | E 41 | 62.878 | 43.361 | 47.433 | 1.00 | 55.88 6 |
| | ATOM | 6894 | C | VAL | E 41 | 59.925 | 41.520 | 49.078 | 1.00 | 55.20 6 |
| | ATOM | 6895 | O | VAL | E 41 | 59.230 | 42.094 | 49.908 | 1.00 | 55.44 8 |
| | ATOM | 6896 | N | ASN | E 42 | 60.042 | 40.204 | 49.025 | 1.00 | 55.58 7 |
| | ATOM | 6897 | CA | ASN | E 42 | 59.381 | 39.350 | 49.995 | 1.00 | 56.97 6 |
| 20 | ATOM | 6898 | CB | ASN | E 42 | 58.077 | 38.794 | 49.430 | 1.00 | 55.95 6 |
| | ATOM | 6899 | CG | ASN | E 42 | 57.220 | 38.135 | 50.490 | 1.00 | 55.31 6 |
| | ATOM | 6900 | OD1 | ASN | E 42 | 57.696 | 37.306 | 51.267 | 1.00 | 56.29 8 |
| | ATOM | 6901 | ND2 | ASN | E 42 | 55.948 | 38.499 | 50.526 | 1.00 | 53.42 7 |
| | ATOM | 6902 | C | ASN | E 42 | 60.360 | 38.222 | 50.241 | 1.00 | 59.68 6 |
| 25 | ATOM | 6903 | O | ASN | E 42 | 60.527 | 37.337 | 49.393 | 1.00 | 60.84 8 |
| | ATOM | 6904 | N | GLU | E 43 | 61.014 | 38.255 | 51.398 | 1.00 | 61.29 7 |
| | ATOM | 6905 | CA | GLU | E 43 | 62.005 | 37.242 | 51.717 | 1.00 | 62.43 6 |
| | ATOM | 6906 | CB | GLU | E 43 | 62.898 | 37.721 | 52.857 | 1.00 | 65.13 6 |
| | ATOM | 6907 | CG | GLU | E 43 | 64.066 | 36.787 | 53.120 | 1.00 | 70.44 6 |
| 30 | ATOM | 6908 | CD | GLU | E 43 | 65.091 | 37.358 | 54.094 | 1.00 | 73.76 6 |
| | ATOM | 6909 | OE1 | GLU | E 43 | 66.010 | 36.601 | 54.486 | 1.00 | 74.81 8 |
| | ATOM | 6910 | OE2 | GLU | E 43 | 64.982 | 38.557 | 54.460 | 1.00 | 74.43 8 |
| | ATOM | 6911 | C | GLU | E 43 | 61.355 | 35.920 | 52.070 | 1.00 | 61.19 6 |
| | ATOM | 6912 | O | GLU | E 43 | 61.977 | 34.861 | 51.958 | 1.00 | 58.53 8 |
| 35 | ATOM | 6913 | N | ILE | E 44 | 60.094 | 35.994 | 52.484 | 1.00 | 61.32 7 |
| | ATOM | 6914 | CA | ILE | E 44 | 59.330 | 34.809 | 52.852 | 1.00 | 61.37 6 |
| | ATOM | 6915 | CB | ILE | E 44 | 57.999 | 35.178 | 53.536 | 1.00 | 62.70 6 |
| | ATOM | 6916 | CG2 | ILE | E 44 | 57.197 | 33.897 | 53.812 | 1.00 | 63.01 6 |
| | ATOM | 6917 | CG1 | ILE | E 44 | 58.258 | 35.946 | 54.836 | 1.00 | 62.78 6 |
| 40 | ATOM | 6918 | CD1 | ILE | E 44 | 58.852 | 35.088 | 55.947 | 1.00 | 63.28 6 |
| | ATOM | 6919 | C | ILE | E 44 | 58.983 | 34.000 | 51.608 | 1.00 | 60.40 6 |
| | ATOM | 6920 | O | ILE | E 44 | 59.114 | 32.774 | 51.592 | 1.00 | 61.80 8 |
| | ATOM | 6921 | N | THR | E 45 | 58.532 | 34.692 | 50.569 | 1.00 | 58.56 7 |
| | ATOM | 6922 | CA | THR | E 45 | 58.149 | 34.033 | 49.326 | 1.00 | 57.28 6 |
| 45 | ATOM | 6923 | CB | THR | E 45 | 56.906 | 34.696 | 48.710 | 1.00 | 56.47 6 |
| | ATOM | 6924 | OG1 | THR | E 45 | 57.189 | 36.074 | 48.443 | 1.00 | 55.94 8 |
| | ATOM | 6925 | CG2 | THR | E 45 | 55.724 | 34.588 | 49.658 | 1.00 | 52.56 6 |
| | ATOM | 6926 | C | THR | E 45 | 59.245 | 34.029 | 48.275 | 1.00 | 55.65 6 |
| | ATOM | 6927 | O | THR | E 45 | 59.120 | 33.357 | 47.262 | 1.00 | 55.71 8 |
| 50 | ATOM | 6928 | N | ASN | E 46 | 60.313 | 34.782 | 48.514 | 1.00 | 55.17 7 |
| | ATOM | 6929 | CA | ASN | E 46 | 61.420 | 34.850 | 47.564 | 1.00 | 54.46 6 |
| | ATOM | 6930 | CB | ASN | E 46 | 62.057 | 33.472 | 47.435 | 1.00 | 54.61 6 |
| | ATOM | 6931 | CG | ASN | E 46 | 63.288 | 33.322 | 48.290 | 1.00 | 56.45 6 |
| | ATOM | 6932 | OD1 | ASN | E 46 | 63.674 | 32.213 | 48.638 | 1.00 | 57.64 8 |
| 55 | ATOM | 6933 | ND2 | ASN | E 46 | 63.922 | 34.436 | 48.621 | 1.00 | 53.06 7 |
| | ATOM | 6934 | C | ASN | E 46 | 60.972 | 35.362 | 46.187 | 1.00 | 54.17 6 |
| | ATOM | 6935 | O | ASN | E 46 | 61.259 | 34.764 | 45.149 | 1.00 | 54.29 8 |
| | ATOM | 6936 | N | GLU | E 47 | 60.267 | 36.482 | 46.191 | 1.00 | 52.96 7 |
| | ATOM | 6937 | CA | GLU | E 47 | 59.769 | 37.074 | 44.970 | 1.00 | 51.83 6 |
| 60 | ATOM | 6938 | CB | GLU | E 47 | 58.247 | 36.956 | 44.926 | 1.00 | 50.20 6 |
| | ATOM | 6939 | CG | GLU | E 47 | 57.750 | 35.530 | 44.856 | 1.00 | 50.29 6 |
| | ATOM | 6940 | CD | GLU | E 47 | 56.236 | 35.438 | 44.877 | 1.00 | 52.98 6 |
| | ATOM | 6941 | OE1 | GLU | E 47 | 55.589 | 36.442 | 44.516 | 1.00 | 50.88 8 |
| | ATOM | 6942 | OE2 | GLU | E 47 | 55.692 | 34.358 | 45.237 | 1.00 | 56.10 8 |
| | ATOM | 6943 | C | GLU | E 47 | 60.186 | 38.534 | 44.919 | 1.00 | 51.43 6 |

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|----|------|------|-----|----------|--------|--------|--------|------|-------|---|--|--|--|--|
| 5 | ATOM | 6944 | O | GLU E 47 | 60.134 | 39.243 | 45.919 | 1.00 | 51.14 | 8 | | | | |
| | ATOM | 6945 | N | VAL E 48 | 60.597 | 38.980 | 43.742 | 1.00 | 51.27 | 7 | | | | |
| | ATOM | 6946 | CA | VAL E 48 | 61.037 | 40.352 | 43.574 | 1.00 | 51.20 | 6 | | | | |
| | ATOM | 6947 | CB | VAL E 48 | 62.554 | 40.402 | 43.276 | 1.00 | 52.39 | 6 | | | | |
| | ATOM | 6948 | CG1 | VAL E 48 | 63.000 | 41.822 | 43.081 | 1.00 | 54.32 | 6 | | | | |
| 10 | ATOM | 6949 | CG2 | VAL E 48 | 63.319 | 39.778 | 44.411 | 1.00 | 53.03 | 6 | | | | |
| | ATOM | 6950 | C | VAL E 48 | 60.290 | 41.062 | 42.452 | 1.00 | 49.53 | 6 | | | | |
| | ATOM | 6951 | O | VAL E 48 | 59.974 | 40.474 | 41.425 | 1.00 | 47.97 | 8 | | | | |
| | ATOM | 6952 | N | ASP E 49 | 60.005 | 42.334 | 42.669 | 1.00 | 47.94 | 7 | | | | |
| | ATOM | 6953 | CA | ASP E 49 | 59.335 | 43.146 | 41.680 | 1.00 | 48.29 | 6 | | | | |
| 15 | ATOM | 6954 | CB | ASP E 49 | 58.107 | 43.795 | 42.290 | 1.00 | 49.64 | 6 | | | | |
| | ATOM | 6955 | CG | ASP E 49 | 57.146 | 44.300 | 41.249 | 1.00 | 50.04 | 6 | | | | |
| | ATOM | 6956 | OD1 | ASP E 49 | 57.596 | 44.853 | 40.228 | 1.00 | 47.78 | 8 | | | | |
| | ATOM | 6957 | OD2 | ASP E 49 | 55.931 | 44.151 | 41.459 | 1.00 | 53.33 | 8 | | | | |
| | ATOM | 6958 | C | ASP E 49 | 60.373 | 44.200 | 41.330 | 1.00 | 48.39 | 6 | | | | |
| 20 | ATOM | 6959 | O | ASP E 49 | 60.644 | 45.101 | 42.118 | 1.00 | 48.55 | 8 | | | | |
| | ATOM | 6960 | N | VAL E 50 | 60.950 | 44.085 | 40.140 | 1.00 | 48.88 | 7 | | | | |
| | ATOM | 6961 | CA | VAL E 50 | 62.011 | 44.988 | 39.718 | 1.00 | 48.55 | 6 | | | | |
| | ATOM | 6962 | CB | VAL E 50 | 63.353 | 44.220 | 39.707 | 1.00 | 50.40 | 6 | | | | |
| | ATOM | 6963 | CG1 | VAL E 50 | 63.428 | 43.303 | 38.492 | 1.00 | 49.66 | 6 | | | | |
| 25 | ATOM | 6964 | CG2 | VAL E 50 | 64.511 | 45.188 | 39.721 | 1.00 | 55.70 | 6 | | | | |
| | ATOM | 6965 | C | VAL E 50 | 61.801 | 45.642 | 38.354 | 1.00 | 47.28 | 6 | | | | |
| | ATOM | 6966 | O | VAL E 50 | 61.057 | 45.134 | 37.523 | 1.00 | 48.34 | 8 | | | | |
| | ATOM | 6967 | N | VAL E 51 | 62.467 | 46.777 | 38.144 | 1.00 | 45.37 | 7 | | | | |
| | ATOM | 6968 | CA | VAL E 51 | 62.407 | 47.540 | 36.896 | 1.00 | 43.25 | 6 | | | | |
| 30 | ATOM | 6969 | CB | VAL E 51 | 61.930 | 48.993 | 37.131 | 1.00 | 41.43 | 6 | | | | |
| | ATOM | 6970 | CG1 | VAL E 51 | 62.118 | 49.820 | 35.865 | 1.00 | 39.28 | 6 | | | | |
| | ATOM | 6971 | CG2 | VAL E 51 | 60.478 | 49.000 | 37.546 | 1.00 | 39.33 | 6 | | | | |
| | ATOM | 6972 | C | VAL E 51 | 63.821 | 47.597 | 36.333 | 1.00 | 44.33 | 6 | | | | |
| | ATOM | 6973 | O | VAL E 51 | 64.764 | 47.841 | 37.078 | 1.00 | 46.78 | 8 | | | | |
| 35 | ATOM | 6974 | N | PHE E 52 | 63.978 | 47.383 | 35.029 | 1.00 | 43.60 | 7 | | | | |
| | ATOM | 6975 | CA | PHE E 52 | 65.304 | 47.416 | 34.430 | 1.00 | 41.93 | 6 | | | | |
| | ATOM | 6976 | CB | PHE E 52 | 65.997 | 46.085 | 34.678 | 1.00 | 41.48 | 6 | | | | |
| | ATOM | 6977 | CG | PHE E 52 | 65.275 | 44.917 | 34.070 | 1.00 | 42.18 | 6 | | | | |
| | ATOM | 6978 | CD1 | PHE E 52 | 65.486 | 44.566 | 32.745 | 1.00 | 41.86 | 6 | | | | |
| 40 | ATOM | 6979 | CD2 | PHE E 52 | 64.347 | 44.200 | 34.809 | 1.00 | 43.51 | 6 | | | | |
| | ATOM | 6980 | CE1 | PHE E 52 | 64.784 | 43.527 | 32.167 | 1.00 | 42.36 | 6 | | | | |
| | ATOM | 6981 | CE2 | PHE E 52 | 63.638 | 43.153 | 34.236 | 1.00 | 45.87 | 6 | | | | |
| | ATOM | 6982 | CZ | PHE E 52 | 63.859 | 42.818 | 32.911 | 1.00 | 43.76 | 6 | | | | |
| | ATOM | 6983 | C | PHE E 52 | 65.239 | 47.675 | 32.933 | 1.00 | 44.18 | 6 | | | | |
| 45 | ATOM | 6984 | O | PHE E 52 | 64.183 | 47.574 | 32.314 | 1.00 | 43.22 | 8 | | | | |
| | ATOM | 6985 | N | TRP E 53 | 66.384 | 48.014 | 32.354 | 1.00 | 46.10 | 7 | | | | |
| | ATOM | 6986 | CA | TRP E 53 | 66.466 | 48.252 | 30.927 | 1.00 | 47.08 | 6 | | | | |
| | ATOM | 6987 | CB | TRP E 53 | 67.367 | 49.431 | 30.614 | 1.00 | 46.54 | 6 | | | | |
| | ATOM | 6988 | CG | TRP E 53 | 66.822 | 50.726 | 31.015 | 1.00 | 49.25 | 6 | | | | |
| 50 | ATOM | 6989 | CD2 | TRP E 53 | 67.510 | 51.972 | 30.991 | 1.00 | 51.55 | 6 | | | | |
| | ATOM | 6990 | CE2 | TRP E 53 | 66.616 | 52.951 | 31.471 | 1.00 | 52.89 | 6 | | | | |
| | ATOM | 6991 | CE3 | TRP E 53 | 68.804 | 52.358 | 30.614 | 1.00 | 53.33 | 6 | | | | |
| | ATOM | 6992 | CD1 | TRP E 53 | 65.577 | 50.980 | 31.486 | 1.00 | 50.42 | 6 | | | | |
| | ATOM | 6993 | NE1 | TRP E 53 | 65.440 | 52.318 | 31.765 | 1.00 | 52.93 | 7 | | | | |
| 55 | ATOM | 6994 | CZ2 | TRP E 53 | 66.969 | 54.299 | 31.589 | 1.00 | 54.65 | 6 | | | | |
| | ATOM | 6995 | CZ3 | TRP E 53 | 69.162 | 53.706 | 30.730 | 1.00 | 55.02 | 6 | | | | |
| | ATOM | 6996 | CH2 | TRP E 53 | 68.245 | 54.658 | 31.215 | 1.00 | 56.13 | 6 | | | | |
| | ATOM | 6997 | C | TRP E 53 | 67.070 | 47.018 | 30.316 | 1.00 | 48.44 | 6 | | | | |
| | ATOM | 6998 | O | TRP E 53 | 68.201 | 46.680 | 30.616 | 1.00 | 50.00 | 8 | | | | |
| 60 | ATOM | 6999 | N | GLN E 54 | 66.313 | 46.342 | 29.465 | 1.00 | 49.02 | 7 | | | | |
| | ATOM | 7000 | CA | GLN E 54 | 66.805 | 45.143 | 28.818 | 1.00 | 49.56 | 6 | | | | |
| | ATOM | 7001 | CB | GLN E 54 | 65.648 | 44.193 | 28.517 | 1.00 | 50.24 | 6 | | | | |
| | ATOM | 7002 | CG | GLN E 54 | 66.076 | 42.837 | 28.017 | 1.00 | 52.86 | 6 | | | | |
| | ATOM | 7003 | CD | GLN E 54 | 65.043 | 41.768 | 28.313 | 1.00 | 57.64 | 6 | | | | |
| | ATOM | 7004 | OE1 | GLN E 54 | 64.668 | 41.564 | 29.465 | 1.00 | 59.29 | 8 | | | | |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 7005 | NE2 | GLN | E | 54 | 64.576 | 41.078 | 27.275 | 1.00 | 58.15 | 7 |
| | ATOM | 7006 | C | GLN | E | 54 | 67.500 | 45.583 | 27.547 | 1.00 | 50.68 | 6 |
| | ATOM | 7007 | O | GLN | E | 54 | 66.972 | 45.458 | 26.446 | 1.00 | 50.31 | 8 |
| | ATOM | 7008 | N | GLN | E | 55 | 68.692 | 46.132 | 27.735 | 1.00 | 53.08 | 7 |
| 5 | ATOM | 7009 | CA | GLN | E | 55 | 69.534 | 46.620 | 26.647 | 1.00 | 55.55 | 6 |
| | ATOM | 7010 | CB | GLN | E | 55 | 70.723 | 47.342 | 27.257 | 1.00 | 57.75 | 6 |
| | ATOM | 7011 | CG | GLN | E | 55 | 71.798 | 47.759 | 26.296 | 1.00 | 65.99 | 6 |
| | ATOM | 7012 | CD | GLN | E | 55 | 72.759 | 48.745 | 26.952 | 1.00 | 70.80 | 6 |
| | ATOM | 7013 | OE1 | GLN | E | 55 | 73.057 | 48.637 | 28.158 | 1.00 | 74.02 | 8 |
| 10 | ATOM | 7014 | NE2 | GLN | E | 55 | 73.245 | 49.710 | 26.175 | 1.00 | 70.33 | 7 |
| | ATOM | 7015 | C | GLN | E | 55 | 69.978 | 45.446 | 25.768 | 1.00 | 54.06 | 6 |
| | ATOM | 7016 | O | GLN | E | 55 | 70.834 | 44.648 | 26.147 | 1.00 | 55.16 | 8 |
| | ATOM | 7017 | N | THR | E | 56 | 69.370 | 45.350 | 24.592 | 1.00 | 51.47 | 7 |
| | ATOM | 7018 | CA | THR | E | 56 | 69.638 | 44.266 | 23.664 | 1.00 | 49.57 | 6 |
| 15 | ATOM | 7019 | CB | THR | E | 56 | 68.340 | 43.527 | 23.323 | 1.00 | 48.99 | 6 |
| | ATOM | 7020 | OG1 | THR | E | 56 | 67.621 | 43.259 | 24.530 | 1.00 | 51.03 | 8 |
| | ATOM | 7021 | CG2 | THR | E | 56 | 68.638 | 42.228 | 22.613 | 1.00 | 48.81 | 6 |
| | ATOM | 7022 | C | THR | E | 56 | 70.245 | 44.780 | 22.374 | 1.00 | 48.56 | 6 |
| | ATOM | 7023 | O | THR | E | 56 | 69.919 | 45.870 | 21.916 | 1.00 | 47.42 | 8 |
| 20 | ATOM | 7024 | N | THR | E | 57 | 71.131 | 43.984 | 21.789 | 1.00 | 48.33 | 7 |
| | ATOM | 7025 | CA | THR | E | 57 | 71.778 | 44.370 | 20.545 | 1.00 | 48.63 | 6 |
| | ATOM | 7026 | CB | THR | E | 57 | 73.079 | 45.153 | 20.803 | 1.00 | 48.38 | 6 |
| | ATOM | 7027 | OG1 | THR | E | 57 | 72.786 | 46.369 | 21.504 | 1.00 | 49.73 | 8 |
| | ATOM | 7028 | CG2 | THR | E | 57 | 73.737 | 45.498 | 19.488 | 1.00 | 53.54 | 6 |
| 25 | ATOM | 7029 | C | THR | E | 57 | 72.115 | 43.162 | 19.688 | 1.00 | 47.10 | 6 |
| | ATOM | 7030 | O | THR | E | 57 | 72.462 | 42.094 | 20.196 | 1.00 | 47.16 | 8 |
| | ATOM | 7031 | N | TRP | E | 58 | 71.996 | 43.337 | 18.382 | 1.00 | 44.64 | 7 |
| | ATOM | 7032 | CA | TRP | E | 58 | 72.302 | 42.272 | 17.443 | 1.00 | 45.43 | 6 |
| | ATOM | 7033 | CB | TRP | E | 58 | 71.217 | 41.185 | 17.463 | 1.00 | 44.32 | 6 |
| 30 | ATOM | 7034 | CG | TRP | E | 58 | 69.901 | 41.590 | 16.907 | 1.00 | 41.75 | 6 |
| | ATOM | 7035 | CD2 | TRP | E | 58 | 68.834 | 42.225 | 17.617 | 1.00 | 41.25 | 6 |
| | ATOM | 7036 | CE2 | TRP | E | 58 | 67.800 | 42.458 | 16.689 | 1.00 | 43.06 | 6 |
| | ATOM | 7037 | CE3 | TRP | E | 58 | 68.653 | 42.622 | 18.948 | 1.00 | 42.08 | 6 |
| | ATOM | 7038 | CD1 | TRP | E | 58 | 69.485 | 41.463 | 15.622 | 1.00 | 39.77 | 6 |
| 35 | ATOM | 7039 | NE1 | TRP | E | 58 | 68.229 | 41.982 | 15.477 | 1.00 | 43.20 | 7 |
| | ATOM | 7040 | CZ2 | TRP | E | 58 | 66.598 | 43.072 | 17.043 | 1.00 | 42.98 | 6 |
| | ATOM | 7041 | CZ3 | TRP | E | 58 | 67.462 | 43.232 | 19.301 | 1.00 | 45.88 | 6 |
| | ATOM | 7042 | CH2 | TRP | E | 58 | 66.447 | 43.451 | 18.347 | 1.00 | 46.11 | 6 |
| | ATOM | 7043 | C | TRP | E | 58 | 72.450 | 42.872 | 16.060 | 1.00 | 46.92 | 6 |
| 40 | ATOM | 7044 | O | TRP | E | 58 | 72.312 | 44.079 | 15.874 | 1.00 | 46.99 | 8 |
| | ATOM | 7045 | N | SER | E | 59 | 72.737 | 42.039 | 15.076 | 1.00 | 49.39 | 7 |
| | ATOM | 7046 | CA | SER | E | 59 | 72.933 | 42.571 | 13.738 | 1.00 | 52.86 | 6 |
| | ATOM | 7047 | CB | SER | E | 59 | 74.423 | 42.477 | 13.382 | 1.00 | 55.16 | 6 |
| | ATOM | 7048 | OG | SER | E | 59 | 74.777 | 43.368 | 12.335 | 1.00 | 59.85 | 8 |
| 45 | ATOM | 7049 | C | SER | E | 59 | 72.093 | 41.873 | 12.673 | 1.00 | 53.08 | 6 |
| | ATOM | 7050 | O | SER | E | 59 | 72.023 | 40.640 | 12.621 | 1.00 | 50.22 | 8 |
| | ATOM | 7051 | N | ASP | E | 60 | 71.461 | 42.685 | 11.833 | 1.00 | 55.39 | 7 |
| | ATOM | 7052 | CA | ASP | E | 60 | 70.616 | 42.206 | 10.743 | 1.00 | 58.98 | 6 |
| | ATOM | 7053 | CB | ASP | E | 60 | 69.144 | 42.502 | 11.027 | 1.00 | 59.87 | 6 |
| 50 | ATOM | 7054 | CG | ASP | E | 60 | 68.214 | 41.871 | 10.006 | 1.00 | 61.83 | 6 |
| | ATOM | 7055 | OD1 | ASP | E | 60 | 68.625 | 41.701 | 8.835 | 1.00 | 62.51 | 8 |
| | ATOM | 7056 | OD2 | ASP | E | 60 | 67.060 | 41.556 | 10.374 | 1.00 | 62.82 | 8 |
| | ATOM | 7057 | C | ASP | E | 60 | 71.041 | 42.975 | 9.508 | 1.00 | 61.07 | 6 |
| | ATOM | 7058 | O | ASP | E | 60 | 70.599 | 44.106 | 9.293 | 1.00 | 60.13 | 8 |
| 55 | ATOM | 7059 | N | ARG | E | 61 | 71.896 | 42.351 | 8.701 | 1.00 | 63.73 | 7 |
| | ATOM | 7060 | CA | ARG | E | 61 | 72.428 | 42.989 | 7.501 | 1.00 | 66.18 | 6 |
| | ATOM | 7061 | CB | ARG | E | 61 | 73.580 | 42.155 | 6.908 | 1.00 | 70.24 | 6 |
| | ATOM | 7062 | CG | ARG | E | 61 | 74.957 | 42.308 | 7.596 | 1.00 | 74.18 | 6 |
| | ATOM | 7063 | CD | ARG | E | 61 | 76.042 | 41.679 | 6.722 | 1.00 | 80.58 | 6 |
| 60 | ATOM | 7064 | NE | ARG | E | 61 | 77.411 | 41.855 | 7.223 | 1.00 | 86.19 | 7 |
| | ATOM | 7065 | CZ | ARG | E | 61 | 78.505 | 41.397 | 6.598 | 1.00 | 88.23 | 6 |

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| | | | | | | -188 | | | | |
|----|------|------|-----|-----|---|------|--------|--------|--------|--------------|
| 5 | ATOM | 7066 | NH1 | ARG | E | 61 | 78.383 | 40.734 | 5.447 | 1.00 88.94 7 |
| | ATOM | 7067 | NH2 | ARG | E | 61 | 79.724 | 41.603 | 7.111 | 1.00 88.58 7 |
| | ATOM | 7068 | C | ARG | E | 61 | 71.404 | 43.289 | 6.414 | 1.00 65.48 6 |
| | ATOM | 7069 | O | ARG | E | 61 | 71.655 | 44.145 | 5.561 | 1.00 65.84 8 |
| | ATOM | 7070 | N | THR | E | 62 | 70.255 | 42.610 | 6.439 | 1.00 64.00 7 |
| | ATOM | 7071 | CA | THR | E | 62 | 69.232 | 42.842 | 5.410 | 1.00 61.93 6 |
| | ATOM | 7072 | CB | THR | E | 62 | 68.113 | 41.764 | 5.439 | 1.00 62.28 6 |
| | ATOM | 7073 | OG1 | THR | E | 62 | 67.367 | 41.879 | 6.652 | 1.00 65.24 8 |
| 10 | ATOM | 7074 | CG2 | THR | E | 62 | 68.707 | 40.361 | 5.372 | 1.00 61.73 6 |
| | ATOM | 7075 | C | THR | E | 62 | 68.602 | 44.218 | 5.595 | 1.00 59.03 6 |
| | ATOM | 7076 | O | THR | E | 62 | 67.827 | 44.676 | 4.761 | 1.00 57.27 8 |
| | ATOM | 7077 | N | LEU | E | 63 | 68.962 | 44.868 | 6.697 | 1.00 57.62 7 |
| 15 | ATOM | 7078 | CA | LEU | E | 63 | 68.461 | 46.200 | 7.029 | 1.00 57.37 6 |
| | ATOM | 7079 | CB | LEU | E | 63 | 68.214 | 46.316 | 8.543 | 1.00 55.66 6 |
| | ATOM | 7080 | CG | LEU | E | 63 | 67.253 | 45.322 | 9.196 | 1.00 55.07 6 |
| | ATOM | 7081 | CD1 | LEU | E | 63 | 67.231 | 45.508 | 10.692 | 1.00 52.03 6 |
| | ATOM | 7082 | CD2 | LEU | E | 63 | 65.875 | 45.519 | 8.612 | 1.00 55.09 6 |
| 20 | ATOM | 7083 | C | LEU | E | 63 | 69.471 | 47.277 | 6.625 | 1.00 57.97 6 |
| | ATOM | 7084 | O | LEU | E | 63 | 69.135 | 48.460 | 6.549 | 1.00 56.59 8 |
| | ATOM | 7085 | N | ALA | E | 64 | 70.715 | 46.862 | 6.389 | 1.00 58.86 7 |
| | ATOM | 7086 | CA | ALA | E | 64 | 71.770 | 47.798 | 6.018 | 1.00 60.30 6 |
| | ATOM | 7087 | CB | ALA | E | 64 | 73.077 | 47.055 | 5.844 | 1.00 58.52 6 |
| | ATOM | 7088 | C | ALA | E | 64 | 71.440 | 48.571 | 4.745 | 1.00 61.25 6 |
| 25 | ATOM | 7089 | O | ALA | E | 64 | 70.814 | 48.041 | 3.830 | 1.00 59.01 8 |
| | ATOM | 7090 | N | TRP | E | 65 | 71.845 | 49.832 | 4.702 | 1.00 63.42 7 |
| | ATOM | 7091 | CA | TRP | E | 65 | 71.619 | 50.631 | 3.514 | 1.00 67.05 6 |
| | ATOM | 7092 | CB | TRP | E | 65 | 70.406 | 51.537 | 3.704 | 1.00 66.45 6 |
| | ATOM | 7093 | CG | TRP | E | 65 | 70.513 | 52.506 | 4.835 | 1.00 66.84 6 |
| 30 | ATOM | 7094 | CD2 | TRP | E | 65 | 70.173 | 52.266 | 6.209 | 1.00 67.35 6 |
| | ATOM | 7095 | CE2 | TRP | E | 65 | 70.352 | 53.488 | 6.904 | 1.00 67.71 6 |
| | ATOM | 7096 | CE3 | TRP | E | 65 | 69.730 | 51.141 | 6.920 | 1.00 65.56 6 |
| | ATOM | 7097 | CD1 | TRP | E | 65 | 70.882 | 53.816 | 4.756 | 1.00 66.32 6 |
| | ATOM | 7098 | NE1 | TRP | E | 65 | 70.785 | 54.415 | 5.993 | 1.00 67.91 7 |
| 35 | ATOM | 7099 | CZ2 | TRP | E | 65 | 70.101 | 53.615 | 8.270 | 1.00 65.59 6 |
| | ATOM | 7100 | CZ3 | TRP | E | 65 | 69.483 | 51.267 | 8.272 | 1.00 64.14 6 |
| | ATOM | 7101 | CH2 | TRP | E | 65 | 69.668 | 52.497 | 8.935 | 1.00 65.02 6 |
| | ATOM | 7102 | C | TRP | E | 65 | 72.874 | 51.449 | 3.253 | 1.00 69.81 6 |
| 40 | ATOM | 7103 | O | TRP | E | 65 | 73.908 | 51.237 | 3.902 | 1.00 70.35 8 |
| | ATOM | 7104 | N | ASN | E | 66 | 72.801 | 52.370 | 2.297 | 1.00 71.64 7 |
| | ATOM | 7105 | CA | ASN | E | 66 | 73.956 | 53.203 | 1.999 | 1.00 72.49 6 |
| | ATOM | 7106 | CB | ASN | E | 66 | 74.174 | 53.318 | 0.486 | 1.00 73.41 6 |
| | ATOM | 7107 | CG | ASN | E | 66 | 75.497 | 53.990 | 0.131 | 1.00 75.13 6 |
| | ATOM | 7108 | OD1 | ASN | E | 66 | 75.513 | 55.081 | -0.456 | 1.00 76.49 8 |
| 45 | ATOM | 7109 | ND2 | ASN | E | 66 | 76.614 | 53.347 | 0.487 | 1.00 73.59 7 |
| | ATOM | 7110 | C | ASN | E | 66 | 73.707 | 54.561 | 2.602 | 1.00 72.73 6 |
| | ATOM | 7111 | O | ASN | E | 66 | 72.930 | 55.361 | 2.068 | 1.00 72.23 8 |
| | ATOM | 7112 | N | SER | E | 67 | 74.367 | 54.810 | 3.726 | 1.00 74.00 7 |
| 50 | ATOM | 7113 | CA | SER | E | 67 | 74.231 | 56.076 | 4.441 | 1.00 76.61 6 |
| | ATOM | 7114 | CB | SER | E | 67 | 74.159 | 55.805 | 5.942 | 1.00 76.40 6 |
| | ATOM | 7115 | OG | SER | E | 67 | 75.161 | 54.878 | 6.307 | 1.00 75.84 8 |
| | ATOM | 7116 | C | SER | E | 67 | 75.378 | 57.041 | 4.150 | 1.00 78.08 6 |
| | ATOM | 7117 | O | SER | E | 67 | 75.512 | 58.093 | 4.807 | 1.00 77.79 8 |
| | ATOM | 7118 | N | SER | E | 68 | 76.199 | 56.678 | 3.162 | 1.00 79.24 7 |
| 55 | ATOM | 7119 | CA | SER | E | 68 | 77.353 | 57.486 | 2.769 | 1.00 79.93 6 |
| | ATOM | 7120 | CB | SER | E | 68 | 78.217 | 56.734 | 1.730 | 1.00 80.16 6 |
| | ATOM | 7121 | OG | SER | E | 68 | 77.535 | 56.523 | 0.495 | 1.00 81.02 8 |
| | ATOM | 7122 | C | SER | E | 68 | 76.896 | 58.835 | 2.219 | 1.00 79.10 6 |
| 60 | ATOM | 7123 | O | SER | E | 68 | 77.586 | 59.471 | 1.411 | 1.00 79.89 8 |
| | ATOM | 7124 | N | HIS | E | 69 | 75.722 | 59.261 | 2.664 | 1.00 77.21 7 |
| | ATOM | 7125 | CA | HIS | E | 69 | 75.176 | 60.529 | 2.247 | 1.00 76.33 6 |
| | ATOM | 7126 | CB | HIS | E | 69 | 75.229 | 60.665 | 0.732 | 1.00 76.74 6 |

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|--|--|
| 5 | ATOM | 7127 | CG | HIS | E | 69 | 75.366 | 62.083 | 0.283 | 1.00 | 77.46 | 6 | | |
| | ATOM | 7128 | CD2 | HIS | E | 69 | 74.568 | 62.857 | -0.491 | 1.00 | 76.01 | 6 | | |
| | ATOM | 7129 | ND1 | HIS | E | 69 | 76.390 | 62.898 | 0.720 | 1.00 | 75.50 | 7 | | |
| | ATOM | 7130 | CE1 | HIS | E | 69 | 76.212 | 64.114 | 0.239 | 1.00 | 74.91 | 6 | | |
| | ATOM | 7131 | NE2 | HIS | E | 69 | 75.115 | 64.117 | -0.497 | 1.00 | 77.04 | 7 | | |
| 10 | ATOM | 7132 | C | HIS | E | 69 | 73.748 | 60.641 | 2.716 | 1.00 | 75.96 | 6 | | |
| | ATOM | 7133 | O | HIS | E | 69 | 72.954 | 61.408 | 2.170 | 1.00 | 75.96 | 8 | | |
| | ATOM | 7134 | N | SER | E | 70 | 73.431 | 59.880 | 3.754 | 1.00 | 75.27 | 7 | | |
| | ATOM | 7135 | CA | SER | E | 70 | 72.086 | 59.867 | 4.308 | 1.00 | 72.77 | 6 | | |
| | ATOM | 7136 | CB | SER | E | 70 | 71.307 | 58.758 | 3.639 | 1.00 | 71.14 | 6 | | |
| 15 | ATOM | 7137 | OG | SER | E | 70 | 72.085 | 57.578 | 3.703 | 1.00 | 68.45 | 8 | | |
| | ATOM | 7138 | C | SER | E | 70 | 72.177 | 59.585 | 5.806 | 1.00 | 72.84 | 6 | | |
| | ATOM | 7139 | O | SER | E | 70 | 73.254 | 59.212 | 6.304 | 1.00 | 73.59 | 8 | | |
| | ATOM | 7140 | N | PRO | E | 71 | 71.065 | 59.789 | 6.550 | 1.00 | 71.65 | 7 | | |
| | ATOM | 7141 | CD | PRO | E | 71 | 69.793 | 60.434 | 6.160 | 1.00 | 70.63 | 6 | | |
| 20 | ATOM | 7142 | CA | PRO | E | 71 | 71.091 | 59.521 | 7.989 | 1.00 | 69.54 | 6 | | |
| | ATOM | 7143 | CB | PRO | E | 71 | 69.627 | 59.649 | 8.376 | 1.00 | 69.50 | 6 | | |
| | ATOM | 7144 | CG | PRO | E | 71 | 69.172 | 60.783 | 7.505 | 1.00 | 69.75 | 6 | | |
| | ATOM | 7145 | C | PRO | E | 71 | 71.611 | 58.104 | 8.128 | 1.00 | 67.45 | 6 | | |
| | ATOM | 7146 | O | PRO | E | 71 | 71.371 | 57.288 | 7.249 | 1.00 | 67.47 | 8 | | |
| 25 | ATOM | 7147 | N | ASP | E | 72 | 72.332 | 57.813 | 9.202 | 1.00 | 65.90 | 7 | | |
| | ATOM | 7148 | CA | ASP | E | 72 | 72.888 | 56.480 | 9.401 | 1.00 | 65.38 | 6 | | |
| | ATOM | 7149 | CB | ASP | E | 72 | 74.336 | 56.595 | 9.864 | 1.00 | 66.99 | 6 | | |
| | ATOM | 7150 | CG | ASP | E | 72 | 74.623 | 57.933 | 10.513 | 1.00 | 69.68 | 6 | | |
| | ATOM | 7151 | OD1 | ASP | E | 72 | 75.809 | 58.349 | 10.511 | 1.00 | 72.85 | 8 | | |
| 30 | ATOM | 7152 | OD2 | ASP | E | 72 | 73.659 | 58.564 | 11.022 | 1.00 | 69.14 | 8 | | |
| | ATOM | 7153 | C | ASP | E | 72 | 72.078 | 55.656 | 10.387 | 1.00 | 64.69 | 6 | | |
| | ATOM | 7154 | O | ASP | E | 72 | 72.273 | 54.438 | 10.492 | 1.00 | 62.72 | 8 | | |
| | ATOM | 7155 | N | GLN | E | 73 | 71.194 | 56.334 | 11.122 | 1.00 | 63.38 | 7 | | |
| | ATOM | 7156 | CA | GLN | E | 73 | 70.291 | 55.692 | 12.073 | 1.00 | 62.59 | 6 | | |
| 35 | ATOM | 7157 | CB | GLN | E | 73 | 70.703 | 55.968 | 13.502 | 1.00 | 63.56 | 6 | | |
| | ATOM | 7158 | CG | GLN | E | 73 | 71.812 | 55.147 | 14.064 | 1.00 | 66.36 | 6 | | |
| | ATOM | 7159 | CD | GLN | E | 73 | 72.073 | 55.601 | 15.478 | 1.00 | 69.74 | 6 | | |
| | ATOM | 7160 | OE1 | GLN | E | 73 | 72.311 | 56.794 | 15.711 | 1.00 | 71.52 | 8 | | |
| | ATOM | 7161 | NE2 | GLN | E | 73 | 72.005 | 54.676 | 16.437 | 1.00 | 70.16 | 7 | | |
| 40 | ATOM | 7162 | C | GLN | E | 73 | 68.850 | 56.189 | 11.932 | 1.00 | 60.94 | 6 | | |
| | ATOM | 7163 | O | GLN | E | 73 | 68.599 | 57.336 | 11.548 | 1.00 | 60.74 | 8 | | |
| | ATOM | 7164 | N | VAL | E | 74 | 67.910 | 55.318 | 12.281 | 1.00 | 57.54 | 7 | | |
| | ATOM | 7165 | CA | VAL | E | 74 | 66.495 | 55.652 | 12.254 | 1.00 | 54.00 | 6 | | |
| | ATOM | 7166 | CB | VAL | E | 74 | 65.857 | 55.296 | 10.901 | 1.00 | 52.88 | 6 | | |
| 45 | ATOM | 7167 | CG1 | VAL | E | 74 | 66.391 | 56.201 | 9.814 | 1.00 | 52.07 | 6 | | |
| | ATOM | 7168 | CG2 | VAL | E | 74 | 66.151 | 53.846 | 10.564 | 1.00 | 53.11 | 6 | | |
| | ATOM | 7169 | C | VAL | E | 74 | 65.816 | 54.844 | 13.349 | 1.00 | 51.46 | 6 | | |
| | ATOM | 7170 | O | VAL | E | 74 | 66.355 | 53.838 | 13.804 | 1.00 | 51.44 | 8 | | |
| | ATOM | 7171 | N | SER | E | 75 | 64.649 | 55.299 | 13.789 | 1.00 | 48.05 | 7 | | |
| 50 | ATOM | 7172 | CA | SER | E | 75 | 63.893 | 54.592 | 14.812 | 1.00 | 45.32 | 6 | | |
| | ATOM | 7173 | CB | SER | E | 75 | 63.222 | 55.583 | 15.761 | 1.00 | 44.86 | 6 | | |
| | ATOM | 7174 | OG | SER | E | 75 | 64.122 | 56.022 | 16.763 | 1.00 | 42.99 | 8 | | |
| | ATOM | 7175 | C | SER | E | 75 | 62.846 | 53.727 | 14.123 | 1.00 | 45.51 | 6 | | |
| | ATOM | 7176 | O | SER | E | 75 | 61.959 | 54.228 | 13.431 | 1.00 | 45.94 | 8 | | |
| 55 | ATOM | 7177 | N | VAL | E | 76 | 62.953 | 52.420 | 14.325 | 1.00 | 44.89 | 7 | | |
| | ATOM | 7178 | CA | VAL | E | 76 | 62.052 | 51.463 | 13.706 | 1.00 | 43.76 | 6 | | |
| | ATOM | 7179 | CB | VAL | E | 76 | 62.857 | 50.400 | 12.943 | 1.00 | 44.31 | 6 | | |
| | ATOM | 7180 | CG1 | VAL | E | 76 | 61.930 | 49.411 | 12.296 | 1.00 | 45.29 | 6 | | |
| | ATOM | 7181 | CG2 | VAL | E | 76 | 63.734 | 51.060 | 11.907 | 1.00 | 45.23 | 6 | | |
| 60 | ATOM | 7182 | C | VAL | E | 76 | 61.169 | 50.751 | 14.718 | 1.00 | 43.81 | 6 | | |
| | ATOM | 7183 | O | VAL | E | 76 | 61.641 | 50.331 | 15.772 | 1.00 | 46.08 | 8 | | |
| | ATOM | 7184 | N | PRO | E | 77 | 59.868 | 50.612 | 14.418 | 1.00 | 41.91 | 7 | | |
| | ATOM | 7185 | CD | PRO | E | 77 | 59.085 | 51.238 | 13.344 | 1.00 | 41.05 | 6 | | |
| | ATOM | 7186 | CA | PRO | E | 77 | 58.987 | 49.923 | 15.360 | 1.00 | 39.46 | 6 | | |
| | ATOM | 7187 | CB | PRO | E | 77 | 57.619 | 50.076 | 14.719 | 1.00 | 39.68 | 6 | | |

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|----|------|------|-----|-----|------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 7188 | CG | PRO | E 77 | 57.736 | 51.362 | 13.981 | 1.00 | 41.25 | 6 |
| | ATOM | 7189 | C | PRO | E 77 | 59.407 | 48.464 | 15.456 | 1.00 | 39.33 | 6 |
| | ATOM | 7190 | O | PRO | E 77 | 59.766 | 47.848 | 14.457 | 1.00 | 39.91 | 8 |
| | ATOM | 7191 | N | ILE | E 78 | 59.368 | 47.929 | 16.665 | 1.00 | 39.53 | 7 |
| | ATOM | 7192 | CA | ILE | E 78 | 59.729 | 46.550 | 16.938 | 1.00 | 39.36 | 6 |
| 10 | ATOM | 7193 | CB | ILE | E 78 | 59.440 | 46.235 | 18.408 | 1.00 | 41.90 | 6 |
| | ATOM | 7194 | CG2 | ILE | E 78 | 59.421 | 44.753 | 18.667 | 1.00 | 44.69 | 6 |
| | ATOM | 7195 | CG1 | ILE | E 78 | 60.512 | 46.887 | 19.259 | 1.00 | 45.61 | 6 |
| | ATOM | 7196 | CD1 | ILE | E 78 | 61.904 | 46.569 | 18.783 | 1.00 | 45.82 | 6 |
| | ATOM | 7197 | C | ILE | E 78 | 59.002 | 45.562 | 16.048 | 1.00 | 39.58 | 6 |
| 15 | ATOM | 7198 | O | ILE | E 78 | 59.556 | 44.550 | 15.645 | 1.00 | 39.79 | 8 |
| | ATOM | 7199 | N | SER | E 79 | 57.755 | 45.870 | 15.729 | 1.00 | 41.50 | 7 |
| | ATOM | 7200 | CA | SER | E 79 | 56.932 | 45.011 | 14.891 | 1.00 | 41.99 | 6 |
| | ATOM | 7201 | CB | SER | E 79 | 55.497 | 45.502 | 14.931 | 1.00 | 40.86 | 6 |
| | ATOM | 7202 | OG | SER | E 79 | 55.441 | 46.876 | 14.633 | 1.00 | 44.60 | 8 |
| 20 | ATOM | 7203 | C | SER | E 79 | 57.370 | 44.887 | 13.441 | 1.00 | 43.24 | 6 |
| | ATOM | 7204 | O | SER | E 79 | 56.883 | 44.020 | 12.730 | 1.00 | 43.62 | 8 |
| | ATOM | 7205 | N | SER | E 80 | 58.278 | 45.750 | 12.996 | 1.00 | 44.61 | 7 |
| | ATOM | 7206 | CA | SER | E 80 | 58.751 | 45.713 | 11.619 | 1.00 | 44.15 | 6 |
| | ATOM | 7207 | CB | SER | E 80 | 58.841 | 47.133 | 11.062 | 1.00 | 43.26 | 6 |
| 25 | ATOM | 7208 | OG | SER | E 80 | 57.568 | 47.744 | 11.017 | 1.00 | 47.92 | 8 |
| | ATOM | 7209 | C | SER | E 80 | 60.110 | 45.033 | 11.482 | 1.00 | 45.19 | 6 |
| | ATOM | 7210 | O | SER | E 80 | 60.661 | 44.963 | 10.387 | 1.00 | 46.20 | 8 |
| | ATOM | 7211 | N | LEU | E 81 | 60.645 | 44.533 | 12.589 | 1.00 | 42.25 | 7 |
| | ATOM | 7212 | CA | LEU | E 81 | 61.949 | 43.891 | 12.577 | 1.00 | 42.76 | 6 |
| 30 | ATOM | 7213 | CB | LEU | E 81 | 62.950 | 44.702 | 13.400 | 1.00 | 41.44 | 6 |
| | ATOM | 7214 | CG | LEU | E 81 | 63.144 | 46.190 | 13.150 | 1.00 | 39.51 | 6 |
| | ATOM | 7215 | CD1 | LEU | E 81 | 63.861 | 46.826 | 14.314 | 1.00 | 38.48 | 6 |
| | ATOM | 7216 | CD2 | LEU | E 81 | 63.908 | 46.367 | 11.891 | 1.00 | 43.00 | 6 |
| | ATOM | 7217 | C | LEU | E 81 | 61.846 | 42.530 | 13.216 | 1.00 | 42.93 | 6 |
| 35 | ATOM | 7218 | O | LEU | E 81 | 60.845 | 42.221 | 13.865 | 1.00 | 47.16 | 8 |
| | ATOM | 7219 | N | TRP | E 82 | 62.880 | 41.715 | 13.028 | 1.00 | 39.63 | 7 |
| | ATOM | 7220 | CA | TRP | E 82 | 62.925 | 40.412 | 13.657 | 1.00 | 38.60 | 6 |
| | ATOM | 7221 | CB | TRP | E 82 | 63.872 | 39.465 | 12.941 | 1.00 | 37.23 | 6 |
| | ATOM | 7222 | CG | TRP | E 82 | 64.186 | 38.241 | 13.753 | 1.00 | 39.34 | 6 |
| 40 | ATOM | 7223 | CD2 | TRP | E 82 | 65.272 | 38.087 | 14.678 | 1.00 | 41.49 | 6 |
| | ATOM | 7224 | CE2 | TRP | E 82 | 65.142 | 36.811 | 15.266 | 1.00 | 40.40 | 6 |
| | ATOM | 7225 | CE3 | TRP | E 82 | 66.344 | 38.909 | 15.071 | 1.00 | 41.39 | 6 |
| | ATOM | 7226 | CD1 | TRP | E 82 | 63.469 | 37.086 | 13.814 | 1.00 | 37.83 | 6 |
| | ATOM | 7227 | NE1 | TRP | E 82 | 64.032 | 36.222 | 14.719 | 1.00 | 40.75 | 7 |
| 45 | ATOM | 7228 | CZ2 | TRP | E 82 | 66.044 | 36.335 | 16.228 | 1.00 | 39.91 | 6 |
| | ATOM | 7229 | CZ3 | TRP | E 82 | 67.237 | 38.436 | 16.025 | 1.00 | 38.98 | 6 |
| | ATOM | 7230 | CH2 | TRP | E 82 | 67.080 | 37.161 | 16.591 | 1.00 | 40.84 | 6 |
| | ATOM | 7231 | C | TRP | E 82 | 63.513 | 40.766 | 14.999 | 1.00 | 38.10 | 6 |
| | ATOM | 7232 | O | TRP | E 82 | 64.356 | 41.636 | 15.086 | 1.00 | 39.18 | 8 |
| 50 | ATOM | 7233 | N | VAL | E 83 | 63.068 | 40.104 | 16.049 | 1.00 | 39.36 | 7 |
| | ATOM | 7234 | CA | VAL | E 83 | 63.578 | 40.395 | 17.367 | 1.00 | 38.27 | 6 |
| | ATOM | 7235 | CB | VAL | E 83 | 62.562 | 41.277 | 18.141 | 1.00 | 39.12 | 6 |
| | ATOM | 7236 | CG1 | VAL | E 83 | 62.919 | 41.352 | 19.596 | 1.00 | 43.60 | 6 |
| | ATOM | 7237 | CG2 | VAL | E 83 | 62.557 | 42.678 | 17.565 | 1.00 | 38.09 | 6 |
| 55 | ATOM | 7238 | C | VAL | E 83 | 63.853 | 39.081 | 18.089 | 1.00 | 37.11 | 6 |
| | ATOM | 7239 | O | VAL | E 83 | 63.154 | 38.098 | 17.896 | 1.00 | 39.80 | 8 |
| | ATOM | 7240 | N | PRO | E 84 | 64.909 | 39.039 | 18.899 | 1.00 | 35.89 | 7 |
| | ATOM | 7241 | CD | PRO | E 84 | 65.921 | 40.088 | 19.075 | 1.00 | 38.94 | 6 |
| | ATOM | 7242 | CA | PRO | E 84 | 65.276 | 37.842 | 19.651 | 1.00 | 35.46 | 6 |
| 60 | ATOM | 7243 | CB | PRO | E 84 | 66.485 | 38.306 | 20.456 | 1.00 | 36.52 | 6 |
| | ATOM | 7244 | CG | PRO | E 84 | 67.087 | 39.306 | 19.600 | 1.00 | 37.91 | 6 |
| | ATOM | 7245 | C | PRO | E 84 | 64.134 | 37.398 | 20.555 | 1.00 | 36.04 | 6 |
| | ATOM | 7246 | O | PRO | E 84 | 63.541 | 38.220 | 21.246 | 1.00 | 34.75 | 8 |
| | ATOM | 7247 | N | ASP | E 85 | 63.839 | 36.103 | 20.565 | 1.00 | 33.87 | 7 |
| | ATOM | 7248 | CA | ASP | E 85 | 62.771 | 35.595 | 21.400 | 1.00 | 35.26 | 6 |

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|----|------|------|-----|----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 7249 | CB | ASP E 85 | 62.150 | 34.350 | 20.779 | 1.00 | 37.18 | 6 |
| | ATOM | 7250 | CG | ASP E 85 | 63.150 | 33.259 | 20.556 | 1.00 | 40.21 | 6 |
| | ATOM | 7251 | OD1 | ASP E 85 | 64.268 | 33.583 | 20.129 | 1.00 | 41.52 | 8 |
| | ATOM | 7252 | OD2 | ASP E 85 | 62.828 | 32.079 | 20.789 | 1.00 | 38.39 | 8 |
| | ATOM | 7253 | C | ASP E 85 | 63.277 | 35.290 | 22.794 | 1.00 | 36.88 | 6 |
| 10 | ATOM | 7254 | O | ASP E 85 | 63.139 | 34.174 | 23.287 | 1.00 | 37.96 | 8 |
| | ATOM | 7255 | N | LEU E 86 | 63.848 | 36.307 | 23.427 | 1.00 | 34.95 | 7 |
| | ATOM | 7256 | CA | LEU E 86 | 64.387 | 36.185 | 24.769 | 1.00 | 36.75 | 6 |
| | ATOM | 7257 | CB | LEU E 86 | 65.211 | 37.414 | 25.116 | 1.00 | 36.06 | 6 |
| | ATOM | 7258 | CG | LEU E 86 | 66.410 | 37.646 | 24.221 | 1.00 | 34.31 | 6 |
| 15 | ATOM | 7259 | CD1 | LEU E 86 | 67.131 | 38.893 | 24.653 | 1.00 | 32.72 | 6 |
| | ATOM | 7260 | CD2 | LEU E 86 | 67.300 | 36.446 | 24.287 | 1.00 | 35.49 | 6 |
| | ATOM | 7261 | C | LEU E 86 | 63.317 | 36.021 | 25.816 | 1.00 | 37.61 | 6 |
| | ATOM | 7262 | O | LEU E 86 | 62.226 | 36.557 | 25.694 | 1.00 | 41.91 | 8 |
| | ATOM | 7263 | N | ALA E 87 | 63.652 | 35.293 | 26.865 | 1.00 | 38.39 | 7 |
| 20 | ATOM | 7264 | CA | ALA E 87 | 62.727 | 35.060 | 27.949 | 1.00 | 39.76 | 6 |
| | ATOM | 7265 | CB | ALA E 87 | 61.950 | 33.766 | 27.692 | 1.00 | 37.37 | 6 |
| | ATOM | 7266 | C | ALA E 87 | 63.510 | 34.959 | 29.255 | 1.00 | 41.61 | 6 |
| | ATOM | 7267 | O | ALA E 87 | 64.583 | 34.372 | 29.288 | 1.00 | 42.91 | 8 |
| | ATOM | 7268 | N | ALA E 88 | 62.989 | 35.550 | 30.323 | 1.00 | 41.72 | 7 |
| 25 | ATOM | 7269 | CA | ALA E 88 | 63.639 | 35.460 | 31.624 | 1.00 | 40.16 | 6 |
| | ATOM | 7270 | CB | ALA E 88 | 63.259 | 36.638 | 32.480 | 1.00 | 38.02 | 6 |
| | ATOM | 7271 | C | ALA E 88 | 63.154 | 34.168 | 32.261 | 1.00 | 41.60 | 6 |
| | ATOM | 7272 | O | ALA E 88 | 62.028 | 34.089 | 32.740 | 1.00 | 43.75 | 8 |
| | ATOM | 7273 | N | TYR E 89 | 64.008 | 33.152 | 32.245 | 1.00 | 43.12 | 7 |
| 30 | ATOM | 7274 | CA | TYR E 89 | 63.691 | 31.832 | 32.793 | 1.00 | 44.73 | 6 |
| | ATOM | 7275 | CB | TYR E 89 | 64.970 | 31.010 | 32.900 | 1.00 | 47.55 | 6 |
| | ATOM | 7276 | CG | TYR E 89 | 65.633 | 30.711 | 31.573 | 1.00 | 53.63 | 6 |
| | ATOM | 7277 | CD1 | TYR E 89 | 66.903 | 30.120 | 31.521 | 1.00 | 54.69 | 6 |
| | ATOM | 7278 | CE1 | TYR E 89 | 67.519 | 29.831 | 30.311 | 1.00 | 56.44 | 6 |
| 35 | ATOM | 7279 | CD2 | TYR E 89 | 64.995 | 31.006 | 30.368 | 1.00 | 56.01 | 6 |
| | ATOM | 7280 | CE2 | TYR E 89 | 65.599 | 30.720 | 29.147 | 1.00 | 58.87 | 6 |
| | ATOM | 7281 | CZ | TYR E 89 | 66.860 | 30.131 | 29.125 | 1.00 | 58.82 | 6 |
| | ATOM | 7282 | OH | TYR E 89 | 67.437 | 29.821 | 27.908 | 1.00 | 64.15 | 8 |
| | ATOM | 7283 | C | TYR E 89 | 62.959 | 31.792 | 34.138 | 1.00 | 44.61 | 6 |
| 40 | ATOM | 7284 | O | TYR E 89 | 62.113 | 30.920 | 34.362 | 1.00 | 43.17 | 8 |
| | ATOM | 7285 | N | ASN E 90 | 63.275 | 32.723 | 35.036 | 1.00 | 43.58 | 7 |
| | ATOM | 7286 | CA | ASN E 90 | 62.621 | 32.729 | 36.338 | 1.00 | 43.92 | 6 |
| | ATOM | 7287 | CB | ASN E 90 | 63.658 | 32.682 | 37.469 | 1.00 | 41.30 | 6 |
| | ATOM | 7288 | CG | ASN E 90 | 64.654 | 33.809 | 37.401 | 1.00 | 40.93 | 6 |
| 45 | ATOM | 7289 | OD1 | ASN E 90 | 65.197 | 34.116 | 36.341 | 1.00 | 40.18 | 8 |
| | ATOM | 7290 | ND2 | ASN E 90 | 64.914 | 34.425 | 38.542 | 1.00 | 42.13 | 7 |
| | ATOM | 7291 | C | ASN E 90 | 61.668 | 33.894 | 36.538 | 1.00 | 45.22 | 6 |
| | ATOM | 7292 | O | ASN E 90 | 61.397 | 34.296 | 37.668 | 1.00 | 45.17 | 8 |
| | ATOM | 7293 | N | ALA E 91 | 61.170 | 34.437 | 35.432 | 1.00 | 46.14 | 7 |
| 50 | ATOM | 7294 | CA | ALA E 91 | 60.207 | 35.526 | 35.482 | 1.00 | 44.27 | 6 |
| | ATOM | 7295 | CB | ALA E 91 | 59.974 | 36.095 | 34.110 | 1.00 | 43.16 | 6 |
| | ATOM | 7296 | C | ALA E 91 | 58.937 | 34.881 | 36.006 | 1.00 | 45.11 | 6 |
| | ATOM | 7297 | O | ALA E 91 | 58.543 | 33.800 | 35.577 | 1.00 | 43.27 | 8 |
| | ATOM | 7298 | N | ILE E 92 | 58.306 | 35.569 | 36.940 | 1.00 | 46.13 | 7 |
| 55 | ATOM | 7299 | CA | ILE E 92 | 57.111 | 35.100 | 37.611 | 1.00 | 45.40 | 6 |
| | ATOM | 7300 | CB | ILE E 92 | 57.301 | 35.365 | 39.123 | 1.00 | 49.00 | 6 |
| | ATOM | 7301 | CG2 | ILE E 92 | 56.517 | 36.598 | 39.568 | 1.00 | 53.30 | 6 |
| | ATOM | 7302 | CG1 | ILE E 92 | 56.883 | 34.165 | 39.929 | 1.00 | 50.53 | 6 |
| | ATOM | 7303 | CD1 | ILE E 92 | 56.902 | 34.482 | 41.419 | 1.00 | 57.12 | 6 |
| 60 | ATOM | 7304 | C | ILE E 92 | 55.863 | 35.805 | 37.060 | 1.00 | 43.27 | 6 |
| | ATOM | 7305 | O | ILE E 92 | 54.745 | 35.458 | 37.395 | 1.00 | 40.97 | 8 |
| | ATOM | 7306 | N | SER E 93 | 56.078 | 36.806 | 36.216 | 1.00 | 42.51 | 7 |
| | ATOM | 7307 | CA | SER E 93 | 55.001 | 37.573 | 35.599 | 1.00 | 41.03 | 6 |
| | ATOM | 7308 | CB | SER E 93 | 54.765 | 38.864 | 36.362 | 1.00 | 40.45 | 6 |
| | ATOM | 7309 | OG | SER E 93 | 55.849 | 39.756 | 36.170 | 1.00 | 40.42 | 8 |

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|----|------|------|-----|-----------|--------|--------|--------|------|---------|
| 5 | ATOM | 7310 | C | SER E 93 | 55.497 | 37.925 | 34.214 | 1.00 | 41.98 6 |
| | ATOM | 7311 | O | SER E 93 | 56.686 | 37.781 | 33.932 | 1.00 | 43.61 8 |
| | ATOM | 7312 | N | LYS E 94 | 54.617 | 38.380 | 33.333 | 1.00 | 41.47 7 |
| | ATOM | 7313 | CA | LYS E 94 | 55.109 | 38.738 | 32.018 | 1.00 | 44.98 6 |
| | ATOM | 7314 | CB | LYS E 94 | 54.037 | 38.561 | 30.942 | 1.00 | 44.95 6 |
| 10 | ATOM | 7315 | CG | LYS E 94 | 52.663 | 39.071 | 31.264 | 1.00 | 48.24 6 |
| | ATOM | 7316 | CD | LYS E 94 | 51.659 | 38.499 | 30.255 | 1.00 | 50.47 6 |
| | ATOM | 7317 | CE | LYS E 94 | 52.173 | 38.628 | 28.822 | 1.00 | 53.56 6 |
| | ATOM | 7318 | NZ | LYS E 94 | 51.218 | 38.125 | 27.795 | 1.00 | 54.79 7 |
| | ATOM | 7319 | C | LYS E 94 | 55.675 | 40.151 | 32.031 | 1.00 | 45.16 6 |
| 15 | ATOM | 7320 | O | LYS E 94 | 55.386 | 40.939 | 32.933 | 1.00 | 46.22 8 |
| | ATOM | 7321 | N | PRO E 95 | 56.514 | 40.481 | 31.038 | 1.00 | 43.95 7 |
| | ATOM | 7322 | CD | PRO E 95 | 56.973 | 39.633 | 29.926 | 1.00 | 42.19 6 |
| | ATOM | 7323 | CA | PRO E 95 | 57.131 | 41.802 | 30.957 | 1.00 | 43.02 6 |
| | ATOM | 7324 | CB | PRO E 95 | 58.076 | 41.671 | 29.768 | 1.00 | 42.81 6 |
| 20 | ATOM | 7325 | CG | PRO E 95 | 58.306 | 40.216 | 29.636 | 1.00 | 42.27 6 |
| | ATOM | 7326 | C | PRO E 95 | 56.162 | 42.939 | 30.761 | 1.00 | 42.70 6 |
| | ATOM | 7327 | O | PRO E 95 | 55.320 | 42.899 | 29.870 | 1.00 | 46.65 8 |
| | ATOM | 7328 | N | GLU E 96 | 56.269 | 43.952 | 31.601 | 1.00 | 40.32 7 |
| | ATOM | 7329 | CA | GLU E 96 | 55.424 | 45.115 | 31.446 | 1.00 | 41.45 6 |
| 25 | ATOM | 7330 | CB | GLU E 96 | 54.910 | 45.635 | 32.797 | 1.00 | 42.90 6 |
| | ATOM | 7331 | CG | GLU E 96 | 53.911 | 46.797 | 32.674 | 1.00 | 47.98 6 |
| | ATOM | 7332 | CD | GLU E 96 | 53.396 | 47.308 | 34.024 | 1.00 | 50.94 6 |
| | ATOM | 7333 | OE1 | GLU E 96 | 53.482 | 46.539 | 35.005 | 1.00 | 53.57 8 |
| | ATOM | 7334 | OE2 | GLU E 96 | 52.894 | 48.462 | 34.102 | 1.00 | 47.79 8 |
| 30 | ATOM | 7335 | C | GLU E 96 | 56.372 | 46.123 | 30.830 | 1.00 | 40.44 6 |
| | ATOM | 7336 | O | GLU E 96 | 57.143 | 46.762 | 31.538 | 1.00 | 42.91 8 |
| | ATOM | 7337 | N | VAL E 97 | 56.348 | 46.227 | 29.506 | 1.00 | 36.63 7 |
| | ATOM | 7338 | CA | VAL E 97 | 57.200 | 47.165 | 28.800 | 1.00 | 34.15 6 |
| | ATOM | 7339 | CB | VAL E 97 | 57.230 | 46.850 | 27.311 | 1.00 | 31.33 6 |
| 35 | ATOM | 7340 | CG1 | VAL E 97 | 58.136 | 47.814 | 26.596 | 1.00 | 31.45 6 |
| | ATOM | 7341 | CG2 | VAL E 97 | 57.708 | 45.444 | 27.113 | 1.00 | 28.98 6 |
| | ATOM | 7342 | C | VAL E 97 | 56.665 | 48.576 | 29.041 | 1.00 | 35.79 6 |
| | ATOM | 7343 | O | VAL E 97 | 55.558 | 48.932 | 28.636 | 1.00 | 35.88 8 |
| | ATOM | 7344 | N | LEU E 98 | 57.474 | 49.378 | 29.714 | 1.00 | 35.63 7 |
| 40 | ATOM | 7345 | CA | LEU E 98 | 57.091 | 50.725 | 30.086 | 1.00 | 36.41 6 |
| | ATOM | 7346 | CB | LEU E 98 | 57.787 | 51.098 | 31.395 | 1.00 | 34.14 6 |
| | ATOM | 7347 | CG | LEU E 98 | 57.676 | 50.176 | 32.598 | 1.00 | 33.56 6 |
| | ATOM | 7348 | CD1 | LEU E 98 | 58.694 | 50.570 | 33.602 | 1.00 | 31.56 6 |
| | ATOM | 7349 | CD2 | LEU E 98 | 56.306 | 50.248 | 33.190 | 1.00 | 33.37 6 |
| 45 | ATOM | 7350 | C | LEU E 98 | 57.400 | 51.793 | 29.058 | 1.00 | 36.97 6 |
| | ATOM | 7351 | O | LEU E 98 | 56.969 | 52.936 | 29.203 | 1.00 | 38.13 8 |
| | ATOM | 7352 | N | THR E 99 | 58.133 | 51.426 | 28.018 | 1.00 | 35.68 7 |
| | ATOM | 7353 | CA | THR E 99 | 58.533 | 52.391 | 27.011 | 1.00 | 34.41 6 |
| | ATOM | 7354 | CB | THR E 99 | 60.067 | 52.547 | 27.032 | 1.00 | 35.73 6 |
| 50 | ATOM | 7355 | OG1 | THR E 99 | 60.683 | 51.265 | 26.850 | 1.00 | 39.59 8 |
| | ATOM | 7356 | CG2 | THR E 99 | 60.517 | 53.122 | 28.355 | 1.00 | 34.05 6 |
| | ATOM | 7357 | C | THR E 99 | 58.098 | 52.084 | 25.589 | 1.00 | 33.50 6 |
| | ATOM | 7358 | O | THR E 99 | 57.696 | 50.969 | 25.283 | 1.00 | 33.37 8 |
| | ATOM | 7359 | N | PRO E 100 | 58.155 | 53.093 | 24.701 | 1.00 | 34.01 7 |
| 55 | ATOM | 7360 | CD | PRO E 100 | 58.424 | 54.514 | 24.975 | 1.00 | 36.06 6 |
| | ATOM | 7361 | CA | PRO E 100 | 57.777 | 52.919 | 23.302 | 1.00 | 33.45 6 |
| | ATOM | 7362 | CB | PRO E 100 | 58.227 | 54.223 | 22.669 | 1.00 | 31.60 6 |
| | ATOM | 7363 | CG | PRO E 100 | 57.906 | 55.190 | 23.725 | 1.00 | 32.57 6 |
| | ATOM | 7364 | C | PRO E 100 | 58.529 | 51.719 | 22.769 | 1.00 | 35.44 6 |
| 60 | ATOM | 7365 | O | PRO E 100 | 59.713 | 51.546 | 23.041 | 1.00 | 35.44 8 |
| | ATOM | 7366 | N | GLN E 101 | 57.844 | 50.868 | 22.029 | 1.00 | 37.12 7 |
| | ATOM | 7367 | CA | GLN E 101 | 58.514 | 49.701 | 21.516 | 1.00 | 38.35 6 |
| | ATOM | 7368 | CB | GLN E 101 | 57.551 | 48.532 | 21.476 | 1.00 | 39.07 6 |
| | ATOM | 7369 | CG | GLN E 101 | 57.398 | 47.921 | 22.845 | 1.00 | 43.00 6 |
| | ATOM | 7370 | CD | GLN E 101 | 56.194 | 47.037 | 22.948 | 1.00 | 48.55 6 |

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|------|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 7371 | OE1 | GLN | E | 101 | 56.055 | 46.068 | 22.194 | 1.00 | 50.74 | 8 |
| | ATOM | 7372 | NE2 | GLN | E | 101 | 55.298 | 47.359 | 23.885 | 1.00 | 48.45 | 7 |
| | ATOM | 7373 | C | GLN | E | 101 | 59.146 | 49.950 | 20.181 | 1.00 | 37.98 | 6 |
| | ATOM | 7374 | O | GLN | E | 101 | 58.749 | 49.374 | 19.177 | 1.00 | 36.86 | 8 |
| | ATOM | 7375 | N | LEU | E | 102 | 60.153 | 50.825 | 20.213 | 1.00 | 39.66 | 7 |
| 10 | ATOM | 7376 | CA | LEU | E | 102 | 60.936 | 51.230 | 19.046 | 1.00 | 38.89 | 6 |
| | ATOM | 7377 | CB | LEU | E | 102 | 60.911 | 52.749 | 18.880 | 1.00 | 36.07 | 6 |
| | ATOM | 7378 | CG | LEU | E | 102 | 59.545 | 53.416 | 18.766 | 1.00 | 36.30 | 6 |
| | ATOM | 7379 | CD1 | LEU | E | 102 | 59.712 | 54.906 | 18.615 | 1.00 | 37.57 | 6 |
| | ATOM | 7380 | CD2 | LEU | E | 102 | 58.809 | 52.853 | 17.571 | 1.00 | 37.42 | 6 |
| 15 | ATOM | 7381 | C | LEU | E | 102 | 62.374 | 50.791 | 19.207 | 1.00 | 37.90 | 6 |
| | ATOM | 7382 | O | LEU | E | 102 | 62.909 | 50.784 | 20.312 | 1.00 | 40.06 | 8 |
| | ATOM | 7383 | N | ALA | E | 103 | 62.995 | 50.408 | 18.102 | 1.00 | 37.36 | 7 |
| | ATOM | 7384 | CA | ALA | E | 103 | 64.395 | 50.007 | 18.127 | 1.00 | 38.78 | 6 |
| | ATOM | 7385 | CB | ALA | E | 103 | 64.577 | 48.634 | 17.504 | 1.00 | 37.72 | 6 |
| 20 | ATOM | 7386 | C | ALA | E | 103 | 65.193 | 51.039 | 17.351 | 1.00 | 38.02 | 6 |
| | ATOM | 7387 | O | ALA | E | 103 | 64.645 | 51.890 | 16.666 | 1.00 | 38.29 | 8 |
| | ATOM | 7388 | N | ARG | E | 104 | 66.500 | 50.969 | 17.469 | 1.00 | 40.78 | 7 |
| | ATOM | 7389 | CA | ARG | E | 104 | 67.344 | 51.911 | 16.770 | 1.00 | 44.75 | 6 |
| | ATOM | 7390 | CB | ARG | E | 104 | 68.258 | 52.612 | 17.771 | 1.00 | 44.40 | 6 |
| 25 | ATOM | 7391 | CG | ARG | E | 104 | 68.873 | 53.873 | 17.251 | 1.00 | 45.66 | 6 |
| | ATOM | 7392 | CD | ARG | E | 104 | 67.868 | 54.956 | 16.983 | 1.00 | 43.79 | 6 |
| | ATOM | 7393 | NE | ARG | E | 104 | 68.570 | 56.118 | 16.456 | 1.00 | 46.54 | 7 |
| | ATOM | 7394 | CZ | ARG | E | 104 | 68.008 | 57.289 | 16.175 | 1.00 | 46.54 | 6 |
| | ATOM | 7395 | NH1 | ARG | E | 104 | 66.711 | 57.493 | 16.365 | 1.00 | 47.66 | 7 |
| 30 | ATOM | 7396 | NH2 | ARG | E | 104 | 68.760 | 58.266 | 15.698 | 1.00 | 49.69 | 7 |
| | ATOM | 7397 | C | ARG | E | 104 | 68.142 | 51.099 | 15.763 | 1.00 | 46.58 | 6 |
| | ATOM | 7398 | O | ARG | E | 104 | 68.775 | 50.105 | 16.119 | 1.00 | 47.46 | 8 |
| | ATOM | 7399 | N | VAL | E | 105 | 68.081 | 51.492 | 14.497 | 1.00 | 48.34 | 7 |
| | ATOM | 7400 | CA | VAL | E | 105 | 68.808 | 50.761 | 13.475 | 1.00 | 49.67 | 6 |
| 35 | ATOM | 7401 | CB | VAL | E | 105 | 67.869 | 50.244 | 12.388 | 1.00 | 49.06 | 6 |
| | ATOM | 7402 | CG1 | VAL | E | 105 | 68.643 | 49.361 | 11.431 | 1.00 | 49.26 | 6 |
| | ATOM | 7403 | CG2 | VAL | E | 105 | 66.731 | 49.478 | 13.010 | 1.00 | 49.99 | 6 |
| | ATOM | 7404 | C | VAL | E | 105 | 69.883 | 51.601 | 12.805 | 1.00 | 51.57 | 6 |
| | ATOM | 7405 | O | VAL | E | 105 | 69.606 | 52.684 | 12.272 | 1.00 | 49.78 | 8 |
| 40 | ATOM | 7406 | N | VAL | E | 106 | 71.109 | 51.077 | 12.834 | 1.00 | 53.67 | 7 |
| | ATOM | 7407 | CA | VAL | E | 106 | 72.265 | 51.738 | 12.232 | 1.00 | 55.11 | 6 |
| | ATOM | 7408 | CB | VAL | E | 106 | 73.537 | 51.409 | 13.009 | 1.00 | 54.77 | 6 |
| | ATOM | 7409 | CG1 | VAL | E | 106 | 74.666 | 52.300 | 12.539 | 1.00 | 55.46 | 6 |
| | ATOM | 7410 | CG2 | VAL | E | 106 | 73.283 | 51.577 | 14.507 | 1.00 | 57.64 | 6 |
| 45 | ATOM | 7411 | C | VAL | E | 106 | 72.428 | 51.253 | 10.795 | 1.00 | 55.88 | 6 |
| | ATOM | 7412 | O | VAL | E | 106 | 72.213 | 50.075 | 10.508 | 1.00 | 57.82 | 8 |
| | ATOM | 7413 | N | SER | E | 107 | 72.812 | 52.153 | 9.897 | 1.00 | 55.80 | 7 |
| | ATOM | 7414 | CA | SER | E | 107 | 72.972 | 51.812 | 8.486 | 1.00 | 55.14 | 6 |
| | ATOM | 7415 | CB | SER | E | 107 | 73.610 | 52.984 | 7.740 | 1.00 | 55.20 | 6 |
| 50 | ATOM | 7416 | OG | SER | E | 107 | 74.708 | 53.503 | 8.470 | 1.00 | 58.75 | 8 |
| | ATOM | 7417 | C | SER | E | 107 | 73.738 | 50.530 | 8.175 | 1.00 | 54.04 | 6 |
| | ATOM | 7418 | O | SER | E | 107 | 73.578 | 49.966 | 7.096 | 1.00 | 52.93 | 8 |
| | ATOM | 7419 | N | ASP | E | 108 | 74.558 | 50.062 | 9.105 | 1.00 | 53.77 | 7 |
| | ATOM | 7420 | CA | ASP | E | 108 | 75.324 | 48.847 | 8.862 | 1.00 | 56.74 | 6 |
| 55 | ATOM | 7421 | CB | ASP | E | 108 | 76.691 | 48.938 | 9.548 | 1.00 | 58.54 | 6 |
| | ATOM | 7422 | CG | ASP | E | 108 | 76.597 | 48.911 | 11.055 | 1.00 | 61.09 | 6 |
| | ATOM | 7423 | OD1 | ASP | E | 108 | 75.653 | 49.522 | 11.599 | 1.00 | 63.34 | 8 |
| | ATOM | 7424 | OD2 | ASP | E | 108 | 77.479 | 48.296 | 11.694 | 1.00 | 61.64 | 8 |
| | ATOM | 7425 | C | ASP | E | 108 | 74.612 | 47.563 | 9.288 | 1.00 | 58.86 | 6 |
| 60 | ATOM | 7426 | O | ASP | E | 108 | 75.213 | 46.484 | 9.278 | 1.00 | 58.05 | 8 |
| | ATOM | 7427 | N | GLY | E | 109 | 73.337 | 47.686 | 9.662 | 1.00 | 60.25 | 7 |
| | ATOM | 7428 | CA | GLY | E | 109 | 72.559 | 46.528 | 10.072 | 1.00 | 60.49 | 6 |
| | ATOM | 7429 | C | GLY | E | 109 | 72.581 | 46.229 | 11.563 | 1.00 | 61.38 | 6 |
| | ATOM | 7430 | O | GLY | E | 109 | 72.031 | 45.211 | 12.011 | 1.00 | 60.99 | 8 |
| | ATOM | 7431 | N | GLU | E | 110 | 73.215 | 47.100 | 12.342 | 1.00 | 61.69 | 7 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|--|--|--|--|--|--|--|
| 5 | ATOM | 7432 | CA | GLU | E | 110 | 73.283 | 46.899 | 13.787 | 1.00 | 61.54 | 6 | | | | | | | |
| | ATOM | 7433 | CB | GLU | E | 110 | 74.432 | 47.720 | 14.391 | 1.00 | 64.16 | 6 | | | | | | | |
| | ATOM | 7434 | CG | GLU | E | 110 | 74.946 | 47.231 | 15.755 | 1.00 | 67.88 | 6 | | | | | | | |
| | ATOM | 7435 | CD | GLU | E | 110 | 75.559 | 45.828 | 15.684 | 1.00 | 72.22 | 6 | | | | | | | |
| | ATOM | 7436 | OE1 | GLU | E | 110 | 75.936 | 45.401 | 14.554 | 1.00 | 72.61 | 8 | | | | | | | |
| 10 | ATOM | 7437 | OE2 | GLU | E | 110 | 75.676 | 45.165 | 16.758 | 1.00 | 70.57 | 8 | | | | | | | |
| | ATOM | 7438 | C | GLU | E | 110 | 71.948 | 47.368 | 14.347 | 1.00 | 60.20 | 6 | | | | | | | |
| | ATOM | 7439 | O | GLU | E | 110 | 71.421 | 48.418 | 13.949 | 1.00 | 59.08 | 8 | | | | | | | |
| | ATOM | 7440 | N | VAL | E | 111 | 71.403 | 46.581 | 15.266 | 1.00 | 57.63 | 7 | | | | | | | |
| | ATOM | 7441 | CA | VAL | E | 111 | 70.116 | 46.893 | 15.885 | 1.00 | 54.53 | 6 | | | | | | | |
| 15 | ATOM | 7442 | CB | VAL | E | 111 | 69.065 | 45.797 | 15.557 | 1.00 | 53.43 | 6 | | | | | | | |
| | ATOM | 7443 | CG1 | VAL | E | 111 | 67.728 | 46.159 | 16.178 | 1.00 | 53.30 | 6 | | | | | | | |
| | ATOM | 7444 | CG2 | VAL | E | 111 | 68.932 | 45.631 | 14.053 | 1.00 | 52.07 | 6 | | | | | | | |
| | ATOM | 7445 | C | VAL | E | 111 | 70.231 | 47.017 | 17.406 | 1.00 | 52.96 | 6 | | | | | | | |
| | ATOM | 7446 | O | VAL | E | 111 | 70.846 | 46.170 | 18.066 | 1.00 | 52.11 | 8 | | | | | | | |
| 20 | ATOM | 7447 | N | LEU | E | 112 | 69.641 | 48.070 | 17.961 | 1.00 | 50.09 | 7 | | | | | | | |
| | ATOM | 7448 | CA | LEU | E | 112 | 69.687 | 48.261 | 19.399 | 1.00 | 50.92 | 6 | | | | | | | |
| | ATOM | 7449 | CB | LEU | E | 112 | 70.546 | 49.468 | 19.770 | 1.00 | 55.28 | 6 | | | | | | | |
| | ATOM | 7450 | CG | LEU | E | 112 | 71.820 | 49.846 | 18.992 | 1.00 | 58.58 | 6 | | | | | | | |
| | ATOM | 7451 | CD1 | LEU | E | 112 | 72.649 | 48.603 | 18.629 | 1.00 | 59.41 | 6 | | | | | | | |
| 25 | ATOM | 7452 | CD2 | LEU | E | 112 | 71.428 | 50.603 | 17.742 | 1.00 | 58.46 | 6 | | | | | | | |
| | ATOM | 7453 | C | LEU | E | 112 | 68.286 | 48.485 | 19.930 | 1.00 | 50.61 | 6 | | | | | | | |
| | ATOM | 7454 | O | LEU | E | 112 | 67.628 | 49.437 | 19.535 | 1.00 | 50.59 | 8 | | | | | | | |
| | ATOM | 7455 | N | TYR | E | 113 | 67.835 | 47.597 | 20.816 | 1.00 | 49.12 | 7 | | | | | | | |
| | ATOM | 7456 | CA | TYR | E | 113 | 66.514 | 47.690 | 21.420 | 1.00 | 46.39 | 6 | | | | | | | |
| 30 | ATOM | 7457 | CB | TYR | E | 113 | 65.635 | 46.500 | 21.003 | 1.00 | 45.58 | 6 | | | | | | | |
| | ATOM | 7458 | CG | TYR | E | 113 | 64.235 | 46.491 | 21.610 | 1.00 | 44.58 | 6 | | | | | | | |
| | ATOM | 7459 | CD1 | TYR | E | 113 | 63.453 | 47.650 | 21.655 | 1.00 | 45.06 | 6 | | | | | | | |
| | ATOM | 7460 | CE1 | TYR | E | 113 | 62.162 | 47.632 | 22.177 | 1.00 | 44.35 | 6 | | | | | | | |
| | ATOM | 7461 | CD2 | TYR | E | 113 | 63.684 | 45.318 | 22.105 | 1.00 | 43.68 | 6 | | | | | | | |
| 35 | ATOM | 7462 | CE2 | TYR | E | 113 | 62.395 | 45.287 | 22.629 | 1.00 | 45.23 | 6 | | | | | | | |
| | ATOM | 7463 | CZ | TYR | E | 113 | 61.633 | 46.444 | 22.663 | 1.00 | 46.53 | 6 | | | | | | | |
| | ATOM | 7464 | OH | TYR | E | 113 | 60.346 | 46.399 | 23.183 | 1.00 | 46.01 | 8 | | | | | | | |
| | ATOM | 7465 | C | TYR | E | 113 | 66.721 | 47.679 | 22.915 | 1.00 | 46.41 | 6 | | | | | | | |
| | ATOM | 7466 | O | TYR | E | 113 | 67.194 | 46.697 | 23.463 | 1.00 | 46.43 | 8 | | | | | | | |
| 40 | ATOM | 7467 | N | MET | E | 114 | 66.363 | 48.774 | 23.572 | 1.00 | 46.91 | 7 | | | | | | | |
| | ATOM | 7468 | CA | MET | E | 114 | 66.539 | 48.880 | 25.011 | 1.00 | 48.35 | 6 | | | | | | | |
| | ATOM | 7469 | CB | MET | E | 114 | 67.635 | 49.889 | 25.315 | 1.00 | 51.44 | 6 | | | | | | | |
| | ATOM | 7470 | CG | MET | E | 114 | 68.053 | 49.906 | 26.737 | 1.00 | 56.27 | 6 | | | | | | | |
| | ATOM | 7471 | SD | MET | E | 114 | 68.981 | 51.368 | 27.017 | 1.00 | 65.32 | 16 | | | | | | | |
| 45 | ATOM | 7472 | CE | MET | E | 114 | 70.586 | 50.862 | 26.425 | 1.00 | 63.97 | 6 | | | | | | | |
| | ATOM | 7473 | C | MET | E | 114 | 65.255 | 49.320 | 25.697 | 1.00 | 48.66 | 6 | | | | | | | |
| | ATOM | 7474 | O | MET | E | 114 | 65.095 | 50.494 | 26.036 | 1.00 | 50.19 | 8 | | | | | | | |
| | ATOM | 7475 | N | PRO | E | 115 | 64.325 | 48.383 | 25.920 | 1.00 | 48.19 | 7 | | | | | | | |
| | ATOM | 7476 | CD | PRO | E | 115 | 64.341 | 46.978 | 25.467 | 1.00 | 47.93 | 6 | | | | | | | |
| 50 | ATOM | 7477 | CA | PRO | E | 115 | 63.056 | 48.702 | 26.572 | 1.00 | 46.04 | 6 | | | | | | | |
| | ATOM | 7478 | CB | PRO | E | 115 | 62.150 | 47.590 | 26.077 | 1.00 | 46.59 | 6 | | | | | | | |
| | ATOM | 7479 | CG | PRO | E | 115 | 63.080 | 46.411 | 26.083 | 1.00 | 45.01 | 6 | | | | | | | |
| | ATOM | 7480 | C | PRO | E | 115 | 63.184 | 48.685 | 28.080 | 1.00 | 44.33 | 6 | | | | | | | |
| | ATOM | 7481 | O | PRO | E | 115 | 63.997 | 47.940 | 28.619 | 1.00 | 44.22 | 8 | | | | | | | |
| 55 | ATOM | 7482 | N | SER | E | 116 | 62.397 | 49.510 | 28.761 | 1.00 | 41.95 | 7 | | | | | | | |
| | ATOM | 7483 | CA | SER | E | 116 | 62.428 | 49.514 | 30.217 | 1.00 | 42.78 | 6 | | | | | | | |
| | ATOM | 7484 | CB | SER | E | 116 | 62.113 | 50.884 | 30.773 | 1.00 | 41.77 | 6 | | | | | | | |
| | ATOM | 7485 | OG | SER | E | 116 | 62.191 | 50.841 | 32.181 | 1.00 | 44.88 | 8 | | | | | | | |
| | ATOM | 7486 | C | SER | E | 116 | 61.344 | 48.533 | 30.643 | 1.00 | 43.69 | 6 | | | | | | | |
| 60 | ATOM | 7487 | O | SER | E | 116 | 60.196 | 48.672 | 30.246 | 1.00 | 46.37 | 8 | | | | | | | |
| | ATOM | 7488 | N | ILE | E | 117 | 61.704 | 47.544 | 31.449 | 1.00 | 42.70 | 7 | | | | | | | |
| | ATOM | 7489 | CA | ILE | E | 117 | 60.751 | 46.534 | 31.851 | 1.00 | 40.36 | 6 | | | | | | | |
| | ATOM | 7490 | CB | ILE | E | 117 | 61.182 | 45.152 | 31.304 | 1.00 | 39.17 | 6 | | | | | | | |
| | ATOM | 7491 | CG2 | ILE | E | 117 | 60.251 | 44.080 | 31.792 | 1.00 | 39.63 | 6 | | | | | | | |
| | ATOM | 7492 | CG1 | ILE | E | 117 | 61.207 | 45.173 | 29.787 | 1.00 | 38.62 | 6 | | | | | | | |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 7493 | CD1 | ILE | E | 117 | 61.883 | 43.985 | 29.185 | 1.00 | 35.74 | 6 |
| | ATOM | 7494 | C | ILE | E | 117 | 60.561 | 46.387 | 33.349 | 1.00 | 43.14 | 6 |
| | ATOM | 7495 | O | ILE | E | 117 | 61.525 | 46.400 | 34.116 | 1.00 | 44.32 | 8 |
| | ATOM | 7496 | N | ARG | E | 118 | 59.305 | 46.266 | 33.768 | 1.00 | 43.03 | 7 |
| 5 | ATOM | 7497 | CA | ARG | E | 118 | 59.014 | 46.009 | 35.170 | 1.00 | 42.46 | 6 |
| | ATOM | 7498 | CB | ARG | E | 118 | 57.907 | 46.897 | 35.710 | 1.00 | 40.98 | 6 |
| | ATOM | 7499 | CG | ARG | E | 118 | 57.537 | 46.484 | 37.113 | 1.00 | 39.32 | 6 |
| | ATOM | 7500 | CD | ARG | E | 118 | 56.671 | 47.482 | 37.827 | 1.00 | 40.32 | 6 |
| | ATOM | 7501 | NE | ARG | E | 118 | 56.321 | 46.985 | 39.155 | 1.00 | 40.46 | 7 |
| 10 | ATOM | 7502 | CZ | ARG | E | 118 | 55.762 | 47.717 | 40.108 | 1.00 | 38.25 | 6 |
| | ATOM | 7503 | NH1 | ARG | E | 118 | 55.485 | 48.991 | 39.899 | 1.00 | 41.07 | 7 |
| | ATOM | 7504 | NH2 | ARG | E | 118 | 55.486 | 47.175 | 41.273 | 1.00 | 37.40 | 7 |
| | ATOM | 7505 | C | ARG | E | 118 | 58.552 | 44.557 | 35.140 | 1.00 | 41.73 | 6 |
| | ATOM | 7506 | O | ARG | E | 118 | 57.738 | 44.185 | 34.309 | 1.00 | 41.59 | 8 |
| 15 | ATOM | 7507 | N | GLN | E | 119 | 59.071 | 43.731 | 36.036 | 1.00 | 42.60 | 7 |
| | ATOM | 7508 | CA | GLN | E | 119 | 58.718 | 42.321 | 36.016 | 1.00 | 43.62 | 6 |
| | ATOM | 7509 | CB | GLN | E | 119 | 59.460 | 41.671 | 34.842 | 1.00 | 41.24 | 6 |
| | ATOM | 7510 | CG | GLN | E | 119 | 59.220 | 40.211 | 34.624 | 1.00 | 40.90 | 6 |
| | ATOM | 7511 | CD | GLN | E | 119 | 59.795 | 39.749 | 33.304 | 1.00 | 40.75 | 6 |
| 20 | ATOM | 7512 | OE1 | GLN | E | 119 | 60.829 | 40.227 | 32.879 | 1.00 | 41.44 | 8 |
| | ATOM | 7513 | NE2 | GLN | E | 119 | 59.126 | 38.807 | 32.654 | 1.00 | 44.30 | 7 |
| | ATOM | 7514 | C | GLN | E | 119 | 59.085 | 41.658 | 37.337 | 1.00 | 44.85 | 6 |
| | ATOM | 7515 | O | GLN | E | 119 | 60.030 | 42.059 | 38.006 | 1.00 | 44.93 | 8 |
| | ATOM | 7516 | N | ARG | E | 120 | 58.326 | 40.649 | 37.724 | 1.00 | 46.59 | 7 |
| 25 | ATOM | 7517 | CA | ARG | E | 120 | 58.612 | 39.958 | 38.969 | 1.00 | 49.63 | 6 |
| | ATOM | 7518 | CB | ARG | E | 120 | 57.327 | 39.657 | 39.722 | 1.00 | 52.24 | 6 |
| | ATOM | 7519 | CG | ARG | E | 120 | 56.514 | 40.879 | 40.037 | 1.00 | 59.37 | 6 |
| | ATOM | 7520 | CD | ARG | E | 120 | 55.730 | 40.641 | 41.301 | 1.00 | 65.41 | 6 |
| | ATOM | 7521 | NE | ARG | E | 120 | 56.517 | 40.896 | 42.518 | 1.00 | 68.76 | 7 |
| 30 | ATOM | 7522 | CZ | ARG | E | 120 | 56.467 | 40.125 | 43.606 | 1.00 | 69.55 | 6 |
| | ATOM | 7523 | NH1 | ARG | E | 120 | 55.687 | 39.045 | 43.617 | 1.00 | 67.60 | 7 |
| | ATOM | 7524 | NH2 | ARG | E | 120 | 57.150 | 40.459 | 44.702 | 1.00 | 69.98 | 7 |
| | ATOM | 7525 | C | ARG | E | 120 | 59.365 | 38.662 | 38.724 | 1.00 | 48.95 | 6 |
| | ATOM | 7526 | O | ARG | E | 120 | 59.187 | 38.013 | 37.692 | 1.00 | 47.74 | 8 |
| 35 | ATOM | 7527 | N | PHE | E | 121 | 60.210 | 38.295 | 39.683 | 1.00 | 47.82 | 7 |
| | ATOM | 7528 | CA | PHE | E | 121 | 60.996 | 37.085 | 39.563 | 1.00 | 46.24 | 6 |
| | ATOM | 7529 | CB | PHE | E | 121 | 62.453 | 37.408 | 39.224 | 1.00 | 42.79 | 6 |
| | ATOM | 7530 | CG | PHE | E | 121 | 62.620 | 38.238 | 38.001 | 1.00 | 43.16 | 6 |
| | ATOM | 7531 | CD1 | PHE | E | 121 | 62.431 | 39.605 | 38.052 | 1.00 | 42.55 | 6 |
| 40 | ATOM | 7532 | CD2 | PHE | E | 121 | 62.945 | 37.651 | 36.793 | 1.00 | 41.67 | 6 |
| | ATOM | 7533 | CE1 | PHE | E | 121 | 62.559 | 40.372 | 36.924 | 1.00 | 44.29 | 6 |
| | ATOM | 7534 | CE2 | PHE | E | 121 | 63.074 | 38.406 | 35.667 | 1.00 | 39.85 | 6 |
| | ATOM | 7535 | CZ | PHE | E | 121 | 62.881 | 39.770 | 35.725 | 1.00 | 43.74 | 6 |
| | ATOM | 7536 | C | PHE | E | 121 | 60.991 | 36.243 | 40.812 | 1.00 | 46.96 | 6 |
| 45 | ATOM | 7537 | O | PHE | E | 121 | 60.663 | 36.708 | 41.902 | 1.00 | 44.85 | 8 |
| | ATOM | 7538 | N | SER | E | 122 | 61.381 | 34.987 | 40.619 | 1.00 | 50.04 | 7 |
| | ATOM | 7539 | CA | SER | E | 122 | 61.509 | 34.019 | 41.691 | 1.00 | 50.97 | 6 |
| | ATOM | 7540 | CB | SER | E | 122 | 60.846 | 32.701 | 41.302 | 1.00 | 50.69 | 6 |
| | ATOM | 7541 | OG | SER | E | 122 | 60.993 | 31.753 | 42.338 | 1.00 | 54.83 | 8 |
| 50 | ATOM | 7542 | C | SER | E | 122 | 63.007 | 33.817 | 41.838 | 1.00 | 51.59 | 6 |
| | ATOM | 7543 | O | SER | E | 122 | 63.648 | 33.274 | 40.947 | 1.00 | 51.83 | 8 |
| | ATOM | 7544 | N | CYS | E | 123 | 63.566 | 34.282 | 42.946 | 1.00 | 53.04 | 7 |
| | ATOM | 7545 | CA | CYS | E | 123 | 65.000 | 34.155 | 43.186 | 1.00 | 55.64 | 6 |
| | ATOM | 7546 | C | CYS | E | 123 | 65.301 | 34.247 | 44.680 | 1.00 | 58.47 | 6 |
| 55 | ATOM | 7547 | O | CYS | E | 123 | 64.390 | 34.401 | 45.501 | 1.00 | 58.89 | 8 |
| | ATOM | 7548 | CB | CYS | E | 123 | 65.757 | 35.249 | 42.425 | 1.00 | 53.82 | 6 |
| | ATOM | 7549 | SG | CYS | E | 123 | 65.215 | 36.927 | 42.881 | 1.00 | 56.41 | 16 |
| | ATOM | 7550 | N | ASP | E | 124 | 66.581 | 34.151 | 45.033 | 1.00 | 61.78 | 7 |
| | ATOM | 7551 | CA | ASP | E | 124 | 66.991 | 34.215 | 46.437 | 1.00 | 63.06 | 6 |
| 60 | ATOM | 7552 | CB | ASP | E | 124 | 68.406 | 33.650 | 46.620 | 1.00 | 63.79 | 6 |
| | ATOM | 7553 | CG | ASP | E | 124 | 68.605 | 33.024 | 47.992 | 1.00 | 64.87 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 7554 | OD1 | ASP | E | 124 | 67.970 | 33.502 | 48.967 | 1.00 | 63.75 | 8 |
| | ATOM | 7555 | OD2 | ASP | E | 124 | 69.396 | 32.058 | 48.094 | 1.00 | 65.17 | 8 |
| | ATOM | 7556 | C | ASP | E | 124 | 66.953 | 35.636 | 47.007 | 1.00 | 63.18 | 6 |
| | ATOM | 7557 | O | ASP | E | 124 | 67.748 | 36.495 | 46.630 | 1.00 | 63.39 | 8 |
| 5 | ATOM | 7558 | N | VAL | E | 125 | 66.031 | 35.857 | 47.936 | 1.00 | 63.67 | 7 |
| | ATOM | 7559 | CA | VAL | E | 125 | 65.869 | 37.152 | 48.586 | 1.00 | 63.68 | 6 |
| | ATOM | 7560 | CB | VAL | E | 125 | 64.370 | 37.506 | 48.710 | 1.00 | 61.88 | 6 |
| | ATOM | 7561 | CG1 | VAL | E | 125 | 64.195 | 38.794 | 49.466 | 1.00 | 58.52 | 6 |
| | ATOM | 7562 | CG2 | VAL | E | 125 | 63.751 | 37.608 | 47.331 | 1.00 | 59.91 | 6 |
| 10 | ATOM | 7563 | C | VAL | E | 125 | 66.501 | 37.157 | 49.987 | 1.00 | 64.88 | 6 |
| | ATOM | 7564 | O | VAL | E | 125 | 66.768 | 38.214 | 50.551 | 1.00 | 66.59 | 8 |
| | ATOM | 7565 | N | SER | E | 126 | 66.745 | 35.975 | 50.544 | 1.00 | 64.96 | 7 |
| | ATOM | 7566 | CA | SER | E | 126 | 67.335 | 35.870 | 51.874 | 1.00 | 64.47 | 6 |
| | ATOM | 7567 | CB | SER | E | 126 | 67.672 | 34.410 | 52.185 | 1.00 | 62.82 | 6 |
| 15 | ATOM | 7568 | OG | SER | E | 126 | 68.617 | 33.901 | 51.267 | 1.00 | 61.35 | 8 |
| | ATOM | 7569 | C | SER | E | 126 | 68.588 | 36.729 | 52.013 | 1.00 | 65.71 | 6 |
| | ATOM | 7570 | O | SER | E | 126 | 69.494 | 36.690 | 51.165 | 1.00 | 65.59 | 8 |
| | ATOM | 7571 | N | GLY | E | 127 | 68.632 | 37.519 | 53.082 | 1.00 | 66.30 | 7 |
| | ATOM | 7572 | CA | GLY | E | 127 | 69.788 | 38.369 | 53.309 | 1.00 | 67.81 | 6 |
| 20 | ATOM | 7573 | C | GLY | E | 127 | 69.595 | 39.800 | 52.848 | 1.00 | 69.06 | 6 |
| | ATOM | 7574 | O | GLY | E | 127 | 70.471 | 40.633 | 53.037 | 1.00 | 69.45 | 8 |
| | ATOM | 7575 | N | VAL | E | 128 | 68.444 | 40.093 | 52.253 | 1.00 | 70.68 | 7 |
| | ATOM | 7576 | CA | VAL | E | 128 | 68.179 | 41.438 | 51.771 | 1.00 | 72.21 | 6 |
| | ATOM | 7577 | CB | VAL | E | 128 | 66.784 | 41.575 | 51.127 | 1.00 | 70.88 | 6 |
| 25 | ATOM | 7578 | CG1 | VAL | E | 128 | 66.771 | 40.882 | 49.794 | 1.00 | 74.99 | 6 |
| | ATOM | 7579 | CG2 | VAL | E | 128 | 65.722 | 40.993 | 52.039 | 1.00 | 69.09 | 6 |
| | ATOM | 7580 | C | VAL | E | 128 | 68.233 | 42.480 | 52.855 | 1.00 | 73.85 | 6 |
| | ATOM | 7581 | O | VAL | E | 128 | 68.855 | 43.525 | 52.678 | 1.00 | 74.59 | 8 |
| | ATOM | 7582 | N | ASP | E | 129 | 67.579 | 42.197 | 53.977 | 1.00 | 75.59 | 7 |
| 30 | ATOM | 7583 | CA | ASP | E | 129 | 67.506 | 43.170 | 55.046 | 1.00 | 77.34 | 6 |
| | ATOM | 7584 | CB | ASP | E | 129 | 66.583 | 42.691 | 56.164 | 1.00 | 78.29 | 6 |
| | ATOM | 7585 | CG | ASP | E | 129 | 65.952 | 43.864 | 56.939 | 1.00 | 80.26 | 6 |
| | ATOM | 7586 | OD1 | ASP | E | 129 | 64.733 | 43.805 | 57.257 | 1.00 | 82.07 | 8 |
| | ATOM | 7587 | OD2 | ASP | E | 129 | 66.674 | 44.848 | 57.231 | 1.00 | 78.55 | 8 |
| 35 | ATOM | 7588 | C | ASP | E | 129 | 68.825 | 43.625 | 55.628 | 1.00 | 78.37 | 6 |
| | ATOM | 7589 | O | ASP | E | 129 | 68.852 | 44.624 | 56.362 | 1.00 | 78.49 | 8 |
| | ATOM | 7590 | N | THR | E | 130 | 69.925 | 42.942 | 55.302 | 1.00 | 79.16 | 7 |
| | ATOM | 7591 | CA | THR | E | 130 | 71.201 | 43.391 | 55.847 | 1.00 | 80.17 | 6 |
| | ATOM | 7592 | CB | THR | E | 130 | 71.162 | 43.351 | 57.393 | 1.00 | 83.36 | 6 |
| 40 | ATOM | 7593 | OG1 | THR | E | 130 | 70.028 | 42.564 | 57.803 | 1.00 | 84.91 | 8 |
| | ATOM | 7594 | CG2 | THR | E | 130 | 71.096 | 44.810 | 57.995 | 1.00 | 82.87 | 6 |
| | ATOM | 7595 | C | THR | E | 130 | 72.505 | 42.731 | 55.445 | 1.00 | 78.82 | 6 |
| | ATOM | 7596 | O | THR | E | 130 | 72.549 | 41.553 | 55.068 | 1.00 | 78.45 | 8 |
| | ATOM | 7597 | N | GLU | E | 131 | 73.564 | 43.537 | 55.572 | 1.00 | 78.85 | 7 |
| 45 | ATOM | 7598 | CA | GLU | E | 131 | 74.961 | 43.153 | 55.353 | 1.00 | 78.23 | 6 |
| | ATOM | 7599 | CB | GLU | E | 131 | 75.292 | 41.900 | 56.187 | 1.00 | 80.76 | 6 |
| | ATOM | 7600 | CG | GLU | E | 131 | 75.507 | 42.176 | 57.686 | 1.00 | 82.62 | 6 |
| | ATOM | 7601 | CD | GLU | E | 131 | 75.241 | 40.955 | 58.543 | 1.00 | 83.46 | 6 |
| | ATOM | 7602 | OE1 | GLU | E | 131 | 75.740 | 39.854 | 58.186 | 1.00 | 83.49 | 8 |
| 50 | ATOM | 7603 | OE2 | GLU | E | 131 | 74.534 | 41.107 | 59.565 | 1.00 | 83.07 | 8 |
| | ATOM | 7604 | C | GLU | E | 131 | 75.434 | 42.931 | 53.943 | 1.00 | 77.11 | 6 |
| | ATOM | 7605 | O | GLU | E | 131 | 75.646 | 43.884 | 53.173 | 1.00 | 75.95 | 8 |
| | ATOM | 7606 | N | SER | E | 132 | 75.658 | 41.652 | 53.650 | 1.00 | 76.20 | 7 |
| | ATOM | 7607 | CA | SER | E | 132 | 76.107 | 41.200 | 52.352 | 1.00 | 75.57 | 6 |
| 55 | ATOM | 7608 | CB | SER | E | 132 | 76.773 | 39.831 | 52.501 | 1.00 | 75.40 | 6 |
| | ATOM | 7609 | OG | SER | E | 132 | 75.896 | 38.911 | 53.122 | 1.00 | 73.45 | 8 |
| | ATOM | 7610 | C | SER | E | 132 | 74.858 | 41.115 | 51.462 | 1.00 | 74.79 | 6 |
| | ATOM | 7611 | O | SER | E | 132 | 74.926 | 40.722 | 50.288 | 1.00 | 76.37 | 8 |
| | ATOM | 7612 | N | GLY | E | 133 | 73.719 | 41.484 | 52.048 | 1.00 | 72.67 | 7 |
| 60 | ATOM | 7613 | CA | GLY | E | 133 | 72.459 | 41.482 | 51.330 | 1.00 | 69.80 | 6 |
| | ATOM | 7614 | C | GLY | E | 133 | 72.127 | 40.179 | 50.631 | 1.00 | 67.70 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 7615 | O | GLY | E | 133 | 72.686 | 39.128 | 50.934 | 1.00 | 67.31 | 8 |
| | ATOM | 7616 | N | ALA | E | 134 | 71.205 | 40.256 | 49.681 | 1.00 | 66.03 | 7 |
| | ATOM | 7617 | CA | ALA | E | 134 | 70.799 | 39.081 | 48.931 | 1.00 | 64.43 | 6 |
| | ATOM | 7618 | CB | ALA | E | 134 | 69.275 | 38.990 | 48.879 | 1.00 | 64.83 | 6 |
| 5 | ATOM | 7619 | C | ALA | E | 134 | 71.363 | 39.108 | 47.512 | 1.00 | 63.34 | 6 |
| | ATOM | 7620 | O | ALA | E | 134 | 71.825 | 40.148 | 47.014 | 1.00 | 61.70 | 8 |
| | ATOM | 7621 | N | THR | E | 135 | 71.339 | 37.944 | 46.875 | 1.00 | 61.78 | 7 |
| | ATOM | 7622 | CA | THR | E | 135 | 71.813 | 37.817 | 45.515 | 1.00 | 61.48 | 6 |
| | ATOM | 7623 | CB | THR | E | 135 | 73.108 | 37.043 | 45.446 | 1.00 | 62.04 | 6 |
| 10 | ATOM | 7624 | OG1 | THR | E | 135 | 74.093 | 37.715 | 46.237 | 1.00 | 63.94 | 8 |
| | ATOM | 7625 | CG2 | THR | E | 135 | 73.590 | 36.970 | 44.012 | 1.00 | 63.05 | 6 |
| | ATOM | 7626 | C | THR | E | 135 | 70.741 | 37.102 | 44.718 | 1.00 | 61.03 | 6 |
| | ATOM | 7627 | O | THR | E | 135 | 70.522 | 35.886 | 44.839 | 1.00 | 59.53 | 8 |
| | ATOM | 7628 | N | CYS | E | 136 | 70.049 | 37.901 | 43.919 | 1.00 | 59.40 | 7 |
| 15 | ATOM | 7629 | CA | CYS | E | 136 | 68.975 | 37.422 | 43.083 | 1.00 | 57.62 | 6 |
| | ATOM | 7630 | C | CYS | E | 136 | 69.530 | 37.254 | 41.669 | 1.00 | 56.65 | 6 |
| | ATOM | 7631 | O | CYS | E | 136 | 69.990 | 38.220 | 41.054 | 1.00 | 54.61 | 8 |
| | ATOM | 7632 | CB | CYS | E | 136 | 67.843 | 38.442 | 43.129 | 1.00 | 55.65 | 6 |
| | ATOM | 7633 | SG | CYS | E | 136 | 66.510 | 38.178 | 41.946 | 1.00 | 55.99 | 16 |
| 20 | ATOM | 7634 | N | ARG | E | 137 | 69.517 | 36.016 | 41.180 | 1.00 | 56.36 | 7 |
| | ATOM | 7635 | CA | ARG | E | 137 | 70.025 | 35.717 | 39.853 | 1.00 | 57.23 | 6 |
| | ATOM | 7636 | CB | ARG | E | 137 | 70.861 | 34.437 | 39.871 | 1.00 | 58.80 | 6 |
| | ATOM | 7637 | CG | ARG | E | 137 | 72.068 | 34.513 | 40.774 | 1.00 | 62.70 | 6 |
| | ATOM | 7638 | CD | ARG | E | 137 | 72.482 | 33.125 | 41.241 | 1.00 | 66.89 | 6 |
| 25 | ATOM | 7639 | NE | ARG | E | 137 | 73.230 | 33.182 | 42.500 | 1.00 | 70.82 | 7 |
| | ATOM | 7640 | CZ | ARG | E | 137 | 74.469 | 33.659 | 42.633 | 1.00 | 71.90 | 6 |
| | ATOM | 7641 | NH1 | ARG | E | 137 | 75.134 | 34.130 | 41.578 | 1.00 | 70.38 | 7 |
| | ATOM | 7642 | NH2 | ARG | E | 137 | 75.042 | 33.674 | 43.832 | 1.00 | 71.22 | 7 |
| | ATOM | 7643 | C | ARG | E | 137 | 68.863 | 35.545 | 38.894 | 1.00 | 56.91 | 6 |
| 30 | ATOM | 7644 | O | ARG | E | 137 | 67.909 | 34.822 | 39.177 | 1.00 | 56.92 | 8 |
| | ATOM | 7645 | N | ILE | E | 138 | 68.970 | 36.215 | 37.754 | 1.00 | 54.63 | 7 |
| | ATOM | 7646 | CA | ILE | E | 138 | 67.966 | 36.175 | 36.716 | 1.00 | 51.98 | 6 |
| | ATOM | 7647 | CB | ILE | E | 138 | 67.432 | 37.587 | 36.468 | 1.00 | 51.76 | 6 |
| | ATOM | 7648 | CG2 | ILE | E | 138 | 66.432 | 37.573 | 35.333 | 1.00 | 49.89 | 6 |
| 35 | ATOM | 7649 | CG1 | ILE | E | 138 | 66.817 | 38.137 | 37.757 | 1.00 | 50.16 | 6 |
| | ATOM | 7650 | CD1 | ILE | E | 138 | 66.476 | 39.606 | 37.681 | 1.00 | 47.06 | 6 |
| | ATOM | 7651 | C | ILE | E | 138 | 68.611 | 35.655 | 35.434 | 1.00 | 52.26 | 6 |
| | ATOM | 7652 | O | ILE | E | 138 | 69.557 | 36.261 | 34.933 | 1.00 | 52.12 | 8 |
| | ATOM | 7653 | N | LYS | E | 139 | 68.105 | 34.542 | 34.901 | 1.00 | 52.70 | 7 |
| 40 | ATOM | 7654 | CA | LYS | E | 139 | 68.656 | 33.961 | 33.667 | 1.00 | 53.32 | 6 |
| | ATOM | 7655 | CB | LYS | E | 139 | 68.877 | 32.455 | 33.822 | 1.00 | 53.63 | 6 |
| | ATOM | 7656 | CG | LYS | E | 139 | 69.732 | 32.075 | 35.013 | 1.00 | 57.59 | 6 |
| | ATOM | 7657 | CD | LYS | E | 139 | 70.150 | 30.612 | 34.967 | 1.00 | 59.76 | 6 |
| | ATOM | 7658 | CE | LYS | E | 139 | 71.183 | 30.363 | 33.869 | 1.00 | 62.51 | 6 |
| 45 | ATOM | 7659 | NZ | LYS | E | 139 | 71.624 | 28.928 | 33.787 | 1.00 | 63.48 | 7 |
| | ATOM | 7660 | C | LYS | E | 139 | 67.738 | 34.187 | 32.480 | 1.00 | 52.42 | 6 |
| | ATOM | 7661 | O | LYS | E | 139 | 66.572 | 33.826 | 32.527 | 1.00 | 52.75 | 8 |
| | ATOM | 7662 | N | ILE | E | 140 | 68.264 | 34.770 | 31.410 | 1.00 | 52.23 | 7 |
| | ATOM | 7663 | CA | ILE | E | 140 | 67.449 | 35.013 | 30.229 | 1.00 | 51.67 | 6 |
| 50 | ATOM | 7664 | CB | ILE | E | 140 | 66.995 | 36.513 | 30.165 | 1.00 | 50.77 | 6 |
| | ATOM | 7665 | CG2 | ILE | E | 140 | 66.543 | 36.974 | 31.546 | 1.00 | 51.60 | 6 |
| | ATOM | 7666 | CG1 | ILE | E | 140 | 68.136 | 37.434 | 29.766 | 1.00 | 52.08 | 6 |
| | ATOM | 7667 | CD1 | ILE | E | 140 | 67.815 | 38.915 | 30.060 | 1.00 | 55.62 | 6 |
| | ATOM | 7668 | C | ILE | E | 140 | 68.145 | 34.594 | 28.935 | 1.00 | 51.13 | 6 |
| 55 | ATOM | 7669 | O | ILE | E | 140 | 69.295 | 34.917 | 28.710 | 1.00 | 49.59 | 8 |
| | ATOM | 7670 | N | GLY | E | 141 | 67.434 | 33.840 | 28.102 | 1.00 | 52.11 | 7 |
| | ATOM | 7671 | CA | GLY | E | 141 | 67.985 | 33.382 | 26.833 | 1.00 | 51.58 | 6 |
| | ATOM | 7672 | C | GLY | E | 141 | 66.884 | 33.089 | 25.826 | 1.00 | 51.56 | 6 |
| | ATOM | 7673 | O | GLY | E | 141 | 65.709 | 33.125 | 26.186 | 1.00 | 52.84 | 8 |
| 60 | ATOM | 7674 | N | SER | E | 142 | 67.245 | 32.807 | 24.573 | 1.00 | 49.52 | 7 |
| | ATOM | 7675 | CA | SER | E | 142 | 66.241 | 32.514 | 23.553 | 1.00 | 46.89 | 6 |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 7676 | CB SER E 142 | 66.883 | 32.177 | 22.214 | 1.00 | 44.37 | 6 |
| | ATOM | 7677 | OG SER E 142 | 65.913 | 31.657 | 21.329 | 1.00 | 40.29 | 8 |
| | ATOM | 7678 | C SER E 142 | 65.386 | 31.346 | 23.997 | 1.00 | 47.72 | 6 |
| | ATOM | 7679 | O SER E 142 | 65.880 | 30.376 | 24.584 | 1.00 | 48.09 | 8 |
| | ATOM | 7680 | N TRP E 143 | 64.097 | 31.439 | 23.701 | 1.00 | 47.51 | 7 |
| 10 | ATOM | 7681 | CA TRP E 143 | 63.165 | 30.406 | 24.101 | 1.00 | 46.17 | 6 |
| | ATOM | 7682 | CB TRP E 143 | 61.780 | 31.025 | 24.327 | 1.00 | 45.01 | 6 |
| | ATOM | 7683 | CG TRP E 143 | 60.808 | 30.096 | 24.968 | 1.00 | 42.92 | 6 |
| | ATOM | 7684 | CD2 TRP E 143 | 60.799 | 29.697 | 26.337 | 1.00 | 41.62 | 6 |
| | ATOM | 7685 | CE2 TRP E 143 | 59.721 | 28.803 | 26.505 | 1.00 | 39.45 | 6 |
| 15 | ATOM | 7686 | CE3 TRP E 143 | 61.601 | 30.008 | 27.442 | 1.00 | 42.26 | 6 |
| | ATOM | 7687 | CD1 TRP E 143 | 59.764 | 29.448 | 24.371 | 1.00 | 41.66 | 6 |
| | ATOM | 7688 | NE1 TRP E 143 | 59.106 | 28.669 | 25.288 | 1.00 | 41.08 | 7 |
| | ATOM | 7689 | CZ2 TRP E 143 | 59.423 | 28.216 | 27.736 | 1.00 | 39.02 | 6 |
| | ATOM | 7690 | CZ3 TRP E 143 | 61.305 | 29.426 | 28.662 | 1.00 | 40.87 | 6 |
| 20 | ATOM | 7691 | CH2 TRP E 143 | 60.223 | 28.540 | 28.799 | 1.00 | 41.01 | 6 |
| | ATOM | 7692 | C TRP E 143 | 63.067 | 29.281 | 23.097 | 1.00 | 46.14 | 6 |
| | ATOM | 7693 | O TRP E 143 | 62.816 | 28.147 | 23.467 | 1.00 | 47.72 | 8 |
| | ATOM | 7694 | N THR E 144 | 63.277 | 29.579 | 21.821 | 1.00 | 46.28 | 7 |
| | ATOM | 7695 | CA THR E 144 | 63.141 | 28.539 | 20.808 | 1.00 | 44.88 | 6 |
| 25 | ATOM | 7696 | CB THR E 144 | 61.961 | 28.863 | 19.859 | 1.00 | 42.99 | 6 |
| | ATOM | 7697 | OG1 THR E 144 | 62.131 | 30.174 | 19.308 | 1.00 | 42.03 | 8 |
| | ATOM | 7698 | CG2 THR E 144 | 60.655 | 28.824 | 20.609 | 1.00 | 40.32 | 6 |
| | ATOM | 7699 | C THR E 144 | 64.378 | 28.276 | 19.969 | 1.00 | 46.55 | 6 |
| | ATOM | 7700 | O THR E 144 | 64.434 | 27.294 | 19.243 | 1.00 | 46.91 | 8 |
| 30 | ATOM | 7701 | N HIS E 145 | 65.367 | 29.151 | 20.060 | 1.00 | 48.37 | 7 |
| | ATOM | 7702 | CA HIS E 145 | 66.576 | 28.973 | 19.275 | 1.00 | 50.06 | 6 |
| | ATOM | 7703 | CB HIS E 145 | 66.937 | 30.265 | 18.541 | 1.00 | 49.35 | 6 |
| | ATOM | 7704 | CG HIS E 145 | 65.947 | 30.669 | 17.492 | 1.00 | 49.26 | 6 |
| | ATOM | 7705 | CD2 HIS E 145 | 65.676 | 30.143 | 16.275 | 1.00 | 49.17 | 6 |
| 35 | ATOM | 7706 | ND1 HIS E 145 | 65.112 | 31.756 | 17.634 | 1.00 | 47.03 | 7 |
| | ATOM | 7707 | CE1 HIS E 145 | 64.371 | 31.883 | 16.548 | 1.00 | 48.38 | 6 |
| | ATOM | 7708 | NE2 HIS E 145 | 64.694 | 30.917 | 15.708 | 1.00 | 50.40 | 7 |
| | ATOM | 7709 | C HIS E 145 | 67.754 | 28.529 | 20.125 | 1.00 | 51.77 | 6 |
| | ATOM | 7710 | O HIS E 145 | 68.096 | 29.153 | 21.129 | 1.00 | 50.03 | 8 |
| 40 | ATOM | 7711 | N HIS E 146 | 68.371 | 27.427 | 19.710 | 1.00 | 55.46 | 7 |
| | ATOM | 7712 | CA HIS E 146 | 69.530 | 26.886 | 20.418 | 1.00 | 57.69 | 6 |
| | ATOM | 7713 | CB HIS E 146 | 69.654 | 25.377 | 20.162 | 1.00 | 56.07 | 6 |
| | ATOM | 7714 | CG HIS E 146 | 69.679 | 25.019 | 18.715 | 1.00 | 56.24 | 6 |
| | ATOM | 7715 | CD2 HIS E 146 | 70.477 | 25.442 | 17.707 | 1.00 | 55.97 | 6 |
| 45 | ATOM | 7716 | ND1 HIS E 146 | 68.798 | 24.121 | 18.157 | 1.00 | 58.10 | 7 |
| | ATOM | 7717 | CE1 HIS E 146 | 69.053 | 24.005 | 16.863 | 1.00 | 58.23 | 6 |
| | ATOM | 7718 | NE2 HIS E 146 | 70.068 | 24.797 | 16.566 | 1.00 | 57.28 | 7 |
| | ATOM | 7719 | C HIS E 146 | 70.801 | 27.612 | 19.971 | 1.00 | 58.37 | 6 |
| | ATOM | 7720 | O HIS E 146 | 70.775 | 28.455 | 19.064 | 1.00 | 59.37 | 8 |
| 50 | ATOM | 7721 | N SER E 147 | 71.908 | 27.269 | 20.618 | 1.00 | 60.00 | 7 |
| | ATOM | 7722 | CA SER E 147 | 73.218 | 27.872 | 20.356 | 1.00 | 60.54 | 6 |
| | ATOM | 7723 | CB SER E 147 | 74.268 | 27.134 | 21.185 | 1.00 | 60.36 | 6 |
| | ATOM | 7724 | OG SER E 147 | 74.082 | 25.728 | 21.071 | 1.00 | 61.90 | 8 |
| | ATOM | 7725 | C SER E 147 | 73.690 | 27.960 | 18.897 | 1.00 | 60.61 | 6 |
| 55 | ATOM | 7726 | O SER E 147 | 74.491 | 28.837 | 18.553 | 1.00 | 60.32 | 8 |
| | ATOM | 7727 | N ARG E 148 | 73.197 | 27.072 | 18.041 | 1.00 | 59.60 | 7 |
| | ATOM | 7728 | CA ARG E 148 | 73.611 | 27.083 | 16.646 | 1.00 | 60.89 | 6 |
| | ATOM | 7729 | CB ARG E 148 | 73.307 | 25.722 | 15.996 | 1.00 | 66.00 | 6 |
| | ATOM | 7730 | CG ARG E 148 | 73.902 | 24.527 | 16.756 | 1.00 | 74.00 | 6 |
| 60 | ATOM | 7731 | CD ARG E 148 | 73.462 | 23.177 | 16.169 | 1.00 | 79.80 | 6 |
| | ATOM | 7732 | NE ARG E 148 | 73.749 | 22.052 | 17.077 | 1.00 | 85.45 | 7 |
| | ATOM | 7733 | CZ ARG E 148 | 74.973 | 21.680 | 17.475 | 1.00 | 86.76 | 6 |
| | ATOM | 7734 | NH1 ARG E 148 | 76.045 | 22.338 | 17.046 | 1.00 | 87.13 | 7 |
| | ATOM | 7735 | NH2 ARG E 148 | 75.130 | 20.650 | 18.306 | 1.00 | 86.87 | 7 |
| | ATOM | 7736 | C ARG E 148 | 72.942 | 28.189 | 15.847 | 1.00 | 59.62 | 6 |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 7737 | O ARG E 148 | 73.418 | 28.564 | 14.766 | 1.00 | 58.11 | 8 | |
| | ATOM | 7738 | N GLU E 149 | 71.836 | 28.707 | 16.384 | 1.00 | 58.68 | 7 | |
| | ATOM | 7739 | CA GLU E 149 | 71.067 | 29.756 | 15.716 | 1.00 | 56.72 | 6 | |
| | ATOM | 7740 | CB GLU E 149 | 69.598 | 29.337 | 15.630 | 1.00 | 55.99 | 6 | |
| | ATOM | 7741 | CG GLU E 149 | 69.435 | 27.854 | 15.335 | 1.00 | 57.25 | 6 | |
| | ATOM | 7742 | CD GLU E 149 | 67.992 | 27.402 | 15.239 | 1.00 | 57.65 | 6 | |
| | ATOM | 7743 | OE1 GLU E 149 | 67.166 | 27.825 | 16.075 | 1.00 | 58.97 | 8 | |
| | ATOM | 7744 | OE2 GLU E 149 | 67.684 | 26.606 | 14.332 | 1.00 | 56.32 | 8 | |
| 10 | ATOM | 7745 | C GLU E 149 | 71.214 | 31.073 | 16.463 | 1.00 | 55.95 | 6 | |
| | ATOM | 7746 | O GLU E 149 | 71.423 | 32.122 | 15.852 | 1.00 | 54.41 | 8 | |
| | ATOM | 7747 | N ILE E 150 | 71.109 | 31.012 | 17.787 | 1.00 | 55.27 | 7 | |
| | ATOM | 7748 | CA ILE E 150 | 71.265 | 32.202 | 18.600 | 1.00 | 54.72 | 6 | |
| 15 | ATOM | 7749 | CB ILE E 150 | 69.922 | 32.686 | 19.227 | 1.00 | 54.60 | 6 | |
| | ATOM | 7750 | CG2 ILE E 150 | 70.190 | 33.711 | 20.339 | 1.00 | 51.29 | 6 | |
| | ATOM | 7751 | CG1 ILE E 150 | 69.051 | 33.354 | 18.167 | 1.00 | 53.90 | 6 | |
| | ATOM | 7752 | CD1 ILE E 150 | 67.738 | 33.855 | 18.709 | 1.00 | 52.06 | 6 | |
| | ATOM | 7753 | C ILE E 150 | 72.238 | 31.954 | 19.728 | 1.00 | 55.47 | 6 | |
| | ATOM | 7754 | O ILE E 150 | 72.226 | 30.898 | 20.361 | 1.00 | 54.39 | 8 | |
| 20 | ATOM | 7755 | N SER E 151 | 73.083 | 32.948 | 19.962 | 1.00 | 56.26 | 7 | |
| | ATOM | 7756 | CA SER E 151 | 74.055 | 32.898 | 21.035 | 1.00 | 59.09 | 6 | |
| | ATOM | 7757 | CB SER E 151 | 75.478 | 32.752 | 20.471 | 1.00 | 59.25 | 6 | |
| | ATOM | 7758 | OG SER E 151 | 75.826 | 33.853 | 19.653 | 1.00 | 59.55 | 8 | |
| | ATOM | 7759 | C SER E 151 | 73.904 | 34.226 | 21.770 | 1.00 | 59.98 | 6 | |
| 25 | ATOM | 7760 | O SER E 151 | 73.793 | 35.283 | 21.139 | 1.00 | 59.94 | 8 | |
| | ATOM | 7761 | N VAL E 152 | 73.878 | 34.172 | 23.096 | 1.00 | 60.88 | 7 | |
| | ATOM | 7762 | CA VAL E 152 | 73.739 | 35.380 | 23.900 | 1.00 | 62.73 | 6 | |
| | ATOM | 7763 | CB VAL E 152 | 72.628 | 35.233 | 24.956 | 1.00 | 61.31 | 6 | |
| | ATOM | 7764 | CG1 VAL E 152 | 71.339 | 34.777 | 24.294 | 1.00 | 58.78 | 6 | |
| | ATOM | 7765 | CG2 VAL E 152 | 73.067 | 34.241 | 26.034 | 1.00 | 62.59 | 6 | |
| 30 | ATOM | 7766 | C VAL E 152 | 75.054 | 35.633 | 24.612 | 1.00 | 64.27 | 6 | |
| | ATOM | 7767 | O VAL E 152 | 75.743 | 34.687 | 24.994 | 1.00 | 63.76 | 8 | |
| | ATOM | 7768 | N ASP E 153 | 75.393 | 36.904 | 24.805 | 1.00 | 66.67 | 7 | |
| | ATOM | 7769 | CA ASP E 153 | 76.650 | 37.261 | 25.456 | 1.00 | 70.32 | 6 | |
| 35 | ATOM | 7770 | CB ASP E 153 | 77.713 | 37.471 | 24.381 | 1.00 | 70.77 | 6 | |
| | ATOM | 7771 | CG ASP E 153 | 77.832 | 36.272 | 23.433 | 1.00 | 74.19 | 6 | |
| | ATOM | 7772 | OD1 ASP E 153 | 78.483 | 35.261 | 23.803 | 1.00 | 75.87 | 8 | |
| | ATOM | 7773 | OD2 ASP E 153 | 77.265 | 36.331 | 22.319 | 1.00 | 73.45 | 8 | |
| | ATOM | 7774 | C ASP E 153 | 76.531 | 38.533 | 26.304 | 1.00 | 72.18 | 6 | |
| 40 | ATOM | 7775 | O ASP E 153 | 75.835 | 39.481 | 25.922 | 1.00 | 72.90 | 8 | |
| | ATOM | 7776 | N PRO E 154 | 77.187 | 38.561 | 27.478 | 1.00 | 73.33 | 7 | |
| | ATOM | 7777 | CD PRO E 154 | 77.671 | 37.398 | 28.243 | 1.00 | 72.54 | 6 | |
| | ATOM | 7778 | CA PRO E 154 | 77.123 | 39.755 | 28.332 | 1.00 | 75.06 | 6 | |
| 45 | ATOM | 7779 | CB PRO E 154 | 77.749 | 39.279 | 29.642 | 1.00 | 74.00 | 6 | |
| | ATOM | 7780 | CG PRO E 154 | 77.389 | 37.823 | 29.676 | 1.00 | 74.05 | 6 | |
| | ATOM | 7781 | C PRO E 154 | 77.911 | 40.901 | 27.688 | 1.00 | 77.63 | 6 | |
| | ATOM | 7782 | O PRO E 154 | 78.502 | 40.717 | 26.620 | 1.00 | 78.05 | 8 | |
| | ATOM | 7783 | N THR E 155 | 77.940 | 42.066 | 28.338 | 1.00 | 81.26 | 7 | |
| 50 | ATOM | 7784 | CA THR E 155 | 78.638 | 43.230 | 27.781 | 1.00 | 85.03 | 6 | |
| | ATOM | 7785 | CB THR E 155 | 77.623 | 44.147 | 27.020 | 1.00 | 83.83 | 6 | |
| | ATOM | 7786 | OG1 THR E 155 | 76.717 | 44.749 | 27.956 | 1.00 | 81.33 | 8 | |
| | ATOM | 7787 | CG2 THR E 155 | 76.815 | 43.341 | 26.020 | 1.00 | 83.47 | 6 | |
| | ATOM | 7788 | C THR E 155 | 79.417 | 44.101 | 28.803 | 1.00 | 88.40 | 6 | |
| | ATOM | 7789 | O THR E 155 | 79.900 | 43.592 | 29.825 | 1.00 | 88.82 | 8 | |
| 55 | ATOM | 7790 | N THR E 156 | 79.527 | 45.405 | 28.487 | 1.00 | 91.48 | 7 | |
| | ATOM | 7791 | CA THR E 156 | 80.206 | 46.443 | 29.288 | 1.00 | 93.55 | 6 | |
| | ATOM | 7792 | CB THR E 156 | 79.615 | 47.854 | 29.002 | 1.00 | 93.31 | 6 | |
| | ATOM | 7793 | OG1 THR E 156 | 79.697 | 48.136 | 27.596 | 1.00 | 92.71 | 8 | |
| 60 | ATOM | 7794 | CG2 THR E 156 | 80.376 | 48.925 | 29.813 | 1.00 | 92.25 | 6 | |
| | ATOM | 7795 | C THR E 156 | 80.165 | 46.249 | 30.803 | 1.00 | 95.69 | 6 | |
| | ATOM | 7796 | O THR E 156 | 79.173 | 46.584 | 31.476 | 1.00 | 95.92 | 8 | |
| | ATOM | 7797 | N GLU E 157 | 81.264 | 45.733 | 31.340 | 1.00 | 97.89 | 7 | |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------------|---|
| 5 | ATOM | 7798 | CA | GLU | E | 157 | 81.365 | 45.481 | 32.776 | 1.00100.21 | 6 |
| | ATOM | 7799 | CB | GLU | E | 157 | 82.361 | 44.343 | 33.018 | 1.00101.17 | 6 |
| | ATOM | 7800 | CG | GLU | E | 157 | 82.198 | 43.190 | 32.046 | 1.00103.80 | 6 |
| | ATOM | 7801 | CD | GLU | E | 157 | 83.222 | 42.107 | 32.296 | 1.00105.78 | 6 |
| | ATOM | 7802 | OE1 | GLU | E | 157 | 84.423 | 42.466 | 32.375 | 1.00105.64 | 8 |
| | ATOM | 7803 | OE2 | GLU | E | 157 | 82.828 | 40.907 | 32.410 | 1.00107.35 | 8 |
| | ATOM | 7804 | C | GLU | E | 157 | 81.817 | 46.729 | 33.550 | 1.00100.48 | 6 |
| | ATOM | 7805 | O | GLU | E | 157 | 81.869 | 46.719 | 34.798 | 1.00100.82 | 8 |
| 10 | ATOM | 7806 | N | ASN | E | 158 | 82.151 | 47.793 | 32.818 | 1.00 99.54 | 7 |
| | ATOM | 7807 | CA | ASN | E | 158 | 82.620 | 49.011 | 33.461 | 1.00 98.41 | 6 |
| | ATOM | 7808 | CB | ASN | E | 158 | 83.235 | 49.953 | 32.426 | 1.00100.23 | 6 |
| | ATOM | 7809 | CG | ASN | E | 158 | 84.338 | 49.283 | 31.604 | 1.00101.57 | 6 |
| 15 | ATOM | 7810 | OD1 | ASN | E | 158 | 85.334 | 48.768 | 32.152 | 1.00100.21 | 8 |
| | ATOM | 7811 | ND2 | ASN | E | 158 | 84.165 | 49.286 | 30.274 | 1.00102.69 | 7 |
| | ATOM | 7812 | C | ASN | E | 158 | 81.456 | 49.701 | 34.156 | 1.00 96.86 | 6 |
| | ATOM | 7813 | O | ASN | E | 158 | 81.185 | 49.443 | 35.341 | 1.00 96.41 | 8 |
| | ATOM | 7814 | N | SER | E | 159 | 80.791 | 50.578 | 33.395 | 1.00 94.72 | 7 |
| | ATOM | 7815 | CA | SER | E | 159 | 79.624 | 51.349 | 33.834 | 1.00 91.39 | 6 |
| 20 | ATOM | 7816 | CB | SER | E | 159 | 78.465 | 51.087 | 32.858 | 1.00 91.87 | 6 |
| | ATOM | 7817 | OG | SER | E | 159 | 78.391 | 49.705 | 32.499 | 1.00 92.44 | 8 |
| | ATOM | 7818 | C | SER | E | 159 | 79.169 | 51.080 | 35.269 | 1.00 88.56 | 6 |
| | ATOM | 7819 | O | SER | E | 159 | 78.823 | 49.947 | 35.614 | 1.00 89.22 | 8 |
| 25 | ATOM | 7820 | N | ASP | E | 160 | 79.171 | 52.119 | 36.102 | 1.00 85.19 | 7 |
| | ATOM | 7821 | CA | ASP | E | 160 | 78.744 | 51.966 | 37.495 | 1.00 81.21 | 6 |
| | ATOM | 7822 | CB | ASP | E | 160 | 78.527 | 53.327 | 38.157 | 1.00 80.51 | 6 |
| | ATOM | 7823 | CG | ASP | E | 160 | 78.005 | 53.194 | 39.574 | 1.00 79.98 | 6 |
| | ATOM | 7824 | OD1 | ASP | E | 160 | 77.424 | 54.174 | 40.079 | 1.00 80.37 | 8 |
| | ATOM | 7825 | OD2 | ASP | E | 160 | 78.184 | 52.104 | 40.178 | 1.00 78.39 | 8 |
| 30 | ATOM | 7826 | C | ASP | E | 160 | 77.426 | 51.202 | 37.525 | 1.00 78.59 | 6 |
| | ATOM | 7827 | O | ASP | E | 160 | 76.427 | 51.669 | 36.959 | 1.00 77.98 | 8 |
| | ATOM | 7828 | N | ASP | E | 161 | 77.427 | 50.043 | 38.185 | 1.00 75.05 | 7 |
| | ATOM | 7829 | CA | ASP | E | 161 | 76.233 | 49.203 | 38.283 | 1.00 71.67 | 6 |
| 35 | ATOM | 7830 | CB | ASP | E | 161 | 76.473 | 48.017 | 39.226 | 1.00 70.39 | 6 |
| | ATOM | 7831 | CG | ASP | E | 161 | 77.428 | 46.994 | 38.641 | 1.00 70.69 | 6 |
| | ATOM | 7832 | OD1 | ASP | E | 161 | 77.389 | 46.782 | 37.416 | 1.00 70.97 | 8 |
| | ATOM | 7833 | OD2 | ASP | E | 161 | 78.211 | 46.386 | 39.400 | 1.00 71.91 | 8 |
| | ATOM | 7834 | C | ASP | E | 161 | 74.968 | 49.931 | 38.732 | 1.00 70.49 | 6 |
| | ATOM | 7835 | O | ASP | E | 161 | 73.864 | 49.439 | 38.514 | 1.00 71.58 | 8 |
| 40 | ATOM | 7836 | N | SER | E | 162 | 75.099 | 51.093 | 39.356 | 1.00 68.11 | 7 |
| | ATOM | 7837 | CA | SER | E | 162 | 73.903 | 51.792 | 39.785 | 1.00 66.58 | 6 |
| | ATOM | 7838 | CB | SER | E | 162 | 73.771 | 51.731 | 41.308 | 1.00 66.49 | 6 |
| | ATOM | 7839 | OG | SER | E | 162 | 74.786 | 52.478 | 41.938 | 1.00 64.63 | 8 |
| 45 | ATOM | 7840 | C | SER | E | 162 | 73.856 | 53.237 | 39.319 | 1.00 65.96 | 6 |
| | ATOM | 7841 | O | SER | E | 162 | 73.250 | 54.088 | 39.972 | 1.00 64.77 | 8 |
| | ATOM | 7842 | N | GLU | E | 163 | 74.475 | 53.514 | 38.178 | 1.00 65.61 | 7 |
| | ATOM | 7843 | CA | GLU | E | 163 | 74.474 | 54.872 | 37.676 | 1.00 67.53 | 6 |
| | ATOM | 7844 | CB | GLU | E | 163 | 75.582 | 55.051 | 36.631 | 1.00 70.35 | 6 |
| | ATOM | 7845 | CG | GLU | E | 163 | 75.237 | 54.661 | 35.213 | 1.00 72.94 | 6 |
| 50 | ATOM | 7846 | CD | GLU | E | 163 | 76.338 | 55.083 | 34.225 | 1.00 76.12 | 6 |
| | ATOM | 7847 | OE1 | GLU | E | 163 | 77.424 | 54.448 | 34.241 | 1.00 77.12 | 8 |
| | ATOM | 7848 | OE2 | GLU | E | 163 | 76.118 | 56.054 | 33.445 | 1.00 76.02 | 8 |
| | ATOM | 7849 | C | GLU | E | 163 | 73.108 | 55.271 | 37.113 | 1.00 66.26 | 6 |
| 55 | ATOM | 7850 | O | GLU | E | 163 | 72.873 | 56.442 | 36.800 | 1.00 64.91 | 8 |
| | ATOM | 7851 | N | TYR | E | 164 | 72.211 | 54.292 | 36.990 | 1.00 66.34 | 7 |
| | ATOM | 7852 | CA | TYR | E | 164 | 70.848 | 54.539 | 36.496 | 1.00 65.02 | 6 |
| | ATOM | 7853 | CB | TYR | E | 164 | 70.555 | 53.716 | 35.235 | 1.00 64.40 | 6 |
| | ATOM | 7854 | CG | TYR | E | 164 | 71.386 | 54.109 | 34.051 | 1.00 64.81 | 6 |
| | ATOM | 7855 | CD1 | TYR | E | 164 | 72.237 | 53.191 | 33.437 | 1.00 64.72 | 6 |
| 60 | ATOM | 7856 | CE1 | TYR | E | 164 | 73.040 | 53.559 | 32.351 | 1.00 65.69 | 6 |
| | ATOM | 7857 | CD2 | TYR | E | 164 | 71.350 | 55.413 | 33.559 | 1.00 67.21 | 6 |
| | ATOM | 7858 | CE2 | TYR | E | 164 | 72.154 | 55.805 | 32.471 | 1.00 67.79 | 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|---------|
| 5 | ATOM | 7859 | CZ | TYR E 164 | 72.994 | 54.867 | 31.867 | 1.00 | 67.33 6 |
| | ATOM | 7860 | OH | TYR E 164 | 73.744 | 55.230 | 30.765 | 1.00 | 67.72 8 |
| | ATOM | 7861 | C | TYR E 164 | 69.831 | 54.174 | 37.574 | 1.00 | 63.42 6 |
| | ATOM | 7862 | O | TYR E 164 | 68.642 | 54.458 | 37.442 | 1.00 | 62.96 8 |
| | ATOM | 7863 | N | PHE E 165 | 70.309 | 53.552 | 38.646 | 1.00 | 60.43 7 |
| 10 | ATOM | 7864 | CA | PHE E 165 | 69.428 | 53.139 | 39.717 | 1.00 | 59.92 6 |
| | ATOM | 7865 | CB | PHE E 165 | 70.208 | 52.378 | 40.776 | 1.00 | 58.36 6 |
| | ATOM | 7866 | CG | PHE E 165 | 69.347 | 51.515 | 41.645 | 1.00 | 58.01 6 |
| | ATOM | 7867 | CD1 | PHE E 165 | 68.674 | 50.427 | 41.110 | 1.00 | 55.31 6 |
| | ATOM | 7868 | CD2 | PHE E 165 | 69.189 | 51.802 | 42.994 | 1.00 | 58.36 6 |
| 15 | ATOM | 7869 | CE1 | PHE E 165 | 67.858 | 49.642 | 41.904 | 1.00 | 56.74 6 |
| | ATOM | 7870 | CE2 | PHE E 165 | 68.368 | 51.016 | 43.804 | 1.00 | 57.34 6 |
| | ATOM | 7871 | CZ | PHE E 165 | 67.703 | 49.939 | 43.260 | 1.00 | 57.55 6 |
| | ATOM | 7872 | C | PHE E 165 | 68.732 | 54.324 | 40.356 | 1.00 | 60.15 6 |
| | ATOM | 7873 | O | PHE E 165 | 69.321 | 55.390 | 40.504 | 1.00 | 62.59 8 |
| 20 | ATOM | 7874 | N | SER E 166 | 67.466 | 54.148 | 40.718 | 1.00 | 59.42 7 |
| | ATOM | 7875 | CA | SER E 166 | 66.724 | 55.222 | 41.357 | 1.00 | 57.86 6 |
| | ATOM | 7876 | CB | SER E 166 | 65.241 | 54.869 | 41.503 | 1.00 | 56.65 6 |
| | ATOM | 7877 | OG | SER E 166 | 64.513 | 55.951 | 42.064 | 1.00 | 53.76 8 |
| | ATOM | 7878 | C | SER E 166 | 67.325 | 55.425 | 42.733 | 1.00 | 56.88 6 |
| 25 | ATOM | 7879 | O | SER E 166 | 67.712 | 54.472 | 43.407 | 1.00 | 55.76 8 |
| | ATOM | 7880 | N | GLN E 167 | 67.406 | 56.677 | 43.142 | 1.00 | 56.96 7 |
| | ATOM | 7881 | CA | GLN E 167 | 67.955 | 57.010 | 44.443 | 1.00 | 58.28 6 |
| | ATOM | 7882 | CB | GLN E 167 | 68.547 | 58.423 | 44.401 | 1.00 | 60.41 6 |
| | ATOM | 7883 | CG | GLN E 167 | 67.549 | 59.465 | 43.941 | 1.00 | 64.41 6 |
| 30 | ATOM | 7884 | CD | GLN E 167 | 68.198 | 60.780 | 43.599 | 1.00 | 66.50 6 |
| | ATOM | 7885 | OE1 | GLN E 167 | 68.795 | 61.433 | 44.458 | 1.00 | 67.54 8 |
| | ATOM | 7886 | NE2 | GLN E 167 | 68.089 | 61.184 | 42.330 | 1.00 | 68.48 7 |
| | ATOM | 7887 | C | GLN E 167 | 66.880 | 56.924 | 45.532 | 1.00 | 57.21 6 |
| | ATOM | 7888 | O | GLN E 167 | 67.196 | 56.835 | 46.720 | 1.00 | 56.91 8 |
| 35 | ATOM | 7889 | N | TYR E 168 | 65.613 | 56.932 | 45.133 | 1.00 | 54.47 7 |
| | ATOM | 7890 | CA | TYR E 168 | 64.550 | 56.877 | 46.111 | 1.00 | 53.18 6 |
| | ATOM | 7891 | CB | TYR E 168 | 63.399 | 57.760 | 45.649 | 1.00 | 53.95 6 |
| | ATOM | 7892 | CG | TYR E 168 | 63.881 | 59.125 | 45.249 | 1.00 | 53.27 6 |
| | ATOM | 7893 | CD1 | TYR E 168 | 64.102 | 59.439 | 43.913 | 1.00 | 54.37 6 |
| 40 | ATOM | 7894 | CE1 | TYR E 168 | 64.625 | 60.672 | 43.541 | 1.00 | 56.01 6 |
| | ATOM | 7895 | CD2 | TYR E 168 | 64.190 | 60.077 | 46.208 | 1.00 | 52.09 6 |
| | ATOM | 7896 | CE2 | TYR E 168 | 64.711 | 61.304 | 45.856 | 1.00 | 55.52 6 |
| | ATOM | 7897 | CZ | TYR E 168 | 64.929 | 61.599 | 44.522 | 1.00 | 57.20 6 |
| | ATOM | 7898 | OH | TYR E 168 | 65.458 | 62.815 | 44.177 | 1.00 | 59.36 8 |
| 45 | ATOM | 7899 | C | TYR E 168 | 64.072 | 55.470 | 46.431 | 1.00 | 52.65 6 |
| | ATOM | 7900 | O | TYR E 168 | 63.131 | 55.282 | 47.189 | 1.00 | 53.48 8 |
| | ATOM | 7901 | N | SER E 169 | 64.735 | 54.479 | 45.861 | 1.00 | 51.93 7 |
| | ATOM | 7902 | CA | SER E 169 | 64.387 | 53.093 | 46.117 | 1.00 | 53.34 6 |
| | ATOM | 7903 | CB | SER E 169 | 65.191 | 52.167 | 45.201 | 1.00 | 53.89 6 |
| 50 | ATOM | 7904 | OG | SER E 169 | 64.945 | 50.807 | 45.514 | 1.00 | 50.40 8 |
| | ATOM | 7905 | C | SER E 169 | 64.686 | 52.726 | 47.567 | 1.00 | 54.98 6 |
| | ATOM | 7906 | O | SER E 169 | 65.636 | 53.225 | 48.162 | 1.00 | 54.67 8 |
| | ATOM | 7907 | N | ARG E 170 | 63.875 | 51.844 | 48.131 | 1.00 | 56.35 7 |
| | ATOM | 7908 | CA | ARG E 170 | 64.075 | 51.404 | 49.500 | 1.00 | 56.22 6 |
| 55 | ATOM | 7909 | CB | ARG E 170 | 62.869 | 50.568 | 49.963 | 1.00 | 57.55 6 |
| | ATOM | 7910 | CG | ARG E 170 | 61.832 | 51.361 | 50.724 | 1.00 | 59.10 6 |
| | ATOM | 7911 | CD | ARG E 170 | 60.436 | 50.785 | 50.587 | 1.00 | 63.93 6 |
| | ATOM | 7912 | NE | ARG E 170 | 60.309 | 49.382 | 50.992 | 1.00 | 67.80 7 |
| | ATOM | 7913 | CZ | ARG E 170 | 59.897 | 48.405 | 50.181 | 1.00 | 68.39 6 |
| 60 | ATOM | 7914 | NH1 | ARG E 170 | 59.577 | 48.664 | 48.916 | 1.00 | 66.05 7 |
| | ATOM | 7915 | NH2 | ARG E 170 | 59.784 | 47.163 | 50.637 | 1.00 | 71.45 7 |
| | ATOM | 7916 | C | ARG E 170 | 65.342 | 50.563 | 49.577 | 1.00 | 56.43 6 |
| | ATOM | 7917 | O | ARG E 170 | 65.878 | 50.334 | 50.666 | 1.00 | 57.41 8 |
| | ATOM | 7918 | N | PHE E 171 | 65.833 | 50.115 | 48.423 | 1.00 | 54.16 7 |
| | ATOM | 7919 | CA | PHE E 171 | 67.011 | 49.265 | 48.403 | 1.00 | 53.05 6 |

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|----|------|------|-----|-----------|--------|--------|--------|------|---------|
| 5 | ATOM | 7920 | CB | PHE E 171 | 66.665 | 47.926 | 47.747 | 1.00 | 51.94 6 |
| | ATOM | 7921 | CG | PHE E 171 | 65.392 | 47.326 | 48.259 | 1.00 | 52.21 6 |
| | ATOM | 7922 | CD1 | PHE E 171 | 64.157 | 47.848 | 47.876 | 1.00 | 54.72 6 |
| | ATOM | 7923 | CD2 | PHE E 171 | 65.416 | 46.288 | 49.180 | 1.00 | 52.12 6 |
| | ATOM | 7924 | CE1 | PHE E 171 | 62.963 | 47.346 | 48.412 | 1.00 | 54.00 6 |
| 10 | ATOM | 7925 | CE2 | PHE E 171 | 64.233 | 45.781 | 49.719 | 1.00 | 52.15 6 |
| | ATOM | 7926 | CZ | PHE E 171 | 63.008 | 46.313 | 49.334 | 1.00 | 53.26 6 |
| | ATOM | 7927 | C | PHE E 171 | 68.181 | 49.909 | 47.698 | 1.00 | 54.03 6 |
| | ATOM | 7928 | O | PHE E 171 | 68.056 | 50.993 | 47.137 | 1.00 | 55.23 8 |
| | ATOM | 7929 | N | GLU E 172 | 69.328 | 49.245 | 47.749 | 1.00 | 55.00 7 |
| 15 | ATOM | 7930 | CA | GLU E 172 | 70.520 | 49.755 | 47.106 | 1.00 | 56.51 6 |
| | ATOM | 7931 | CB | GLU E 172 | 71.385 | 50.513 | 48.120 | 1.00 | 58.70 6 |
| | ATOM | 7932 | CG | GLU E 172 | 71.906 | 49.691 | 49.299 | 1.00 | 63.76 6 |
| | ATOM | 7933 | CD | GLU E 172 | 72.716 | 50.527 | 50.300 | 1.00 | 66.16 6 |
| | ATOM | 7934 | OE1 | GLU E 172 | 73.450 | 51.439 | 49.861 | 1.00 | 67.90 8 |
| 20 | ATOM | 7935 | OE2 | GLU E 172 | 72.635 | 50.266 | 51.526 | 1.00 | 67.48 8 |
| | ATOM | 7936 | C | GLU E 172 | 71.288 | 48.596 | 46.490 | 1.00 | 57.61 6 |
| | ATOM | 7937 | O | GLU E 172 | 71.161 | 47.451 | 46.917 | 1.00 | 57.07 8 |
| | ATOM | 7938 | N | ILE E 173 | 72.077 | 48.891 | 45.470 | 1.00 | 58.83 7 |
| | ATOM | 7939 | CA | ILE E 173 | 72.844 | 47.850 | 44.802 | 1.00 | 60.44 6 |
| 25 | ATOM | 7940 | CB | ILE E 173 | 72.863 | 48.063 | 43.274 | 1.00 | 60.05 6 |
| | ATOM | 7941 | CG2 | ILE E 173 | 73.751 | 47.016 | 42.617 | 1.00 | 60.65 6 |
| | ATOM | 7942 | CG1 | ILE E 173 | 71.439 | 47.999 | 42.722 | 1.00 | 60.27 6 |
| | ATOM | 7943 | CD1 | ILE E 173 | 71.357 | 48.283 | 41.245 | 1.00 | 60.88 6 |
| | ATOM | 7944 | C | ILE E 173 | 74.289 | 47.760 | 45.275 | 1.00 | 60.89 6 |
| 30 | ATOM | 7945 | O | ILE E 173 | 75.011 | 48.752 | 45.342 | 1.00 | 60.64 8 |
| | ATOM | 7946 | N | LEU E 174 | 74.715 | 46.555 | 45.595 | 1.00 | 62.24 7 |
| | ATOM | 7947 | CA | LEU E 174 | 76.079 | 46.360 | 46.019 | 1.00 | 63.64 6 |
| | ATOM | 7948 | CB | LEU E 174 | 76.152 | 45.176 | 46.968 | 1.00 | 62.78 6 |
| | ATOM | 7949 | CG | LEU E 174 | 75.126 | 45.262 | 48.086 | 1.00 | 63.68 6 |
| 35 | ATOM | 7950 | CD1 | LEU E 174 | 75.212 | 44.013 | 48.952 | 1.00 | 63.39 6 |
| | ATOM | 7951 | CD2 | LEU E 174 | 75.367 | 46.538 | 48.896 | 1.00 | 62.58 6 |
| | ATOM | 7952 | C | LEU E 174 | 76.908 | 46.093 | 44.760 | 1.00 | 65.84 6 |
| | ATOM | 7953 | O | LEU E 174 | 77.891 | 46.787 | 44.480 | 1.00 | 67.17 8 |
| | ATOM | 7954 | N | ASP E 175 | 76.494 | 45.102 | 43.979 | 1.00 | 67.20 7 |
| 40 | ATOM | 7955 | CA | ASP E 175 | 77.227 | 44.772 | 42.763 | 1.00 | 67.40 6 |
| | ATOM | 7956 | CB | ASP E 175 | 78.496 | 43.999 | 43.148 | 1.00 | 68.39 6 |
| | ATOM | 7957 | CG | ASP E 175 | 79.385 | 43.673 | 41.961 | 1.00 | 67.83 6 |
| | ATOM | 7958 | OD1 | ASP E 175 | 79.754 | 44.600 | 41.192 | 1.00 | 66.66 8 |
| | ATOM | 7959 | OD2 | ASP E 175 | 79.727 | 42.477 | 41.821 | 1.00 | 67.72 8 |
| 45 | ATOM | 7960 | C | ASP E 175 | 76.358 | 43.960 | 41.803 | 1.00 | 67.16 6 |
| | ATOM | 7961 | O | ASP E 175 | 75.405 | 43.291 | 42.216 | 1.00 | 66.38 8 |
| | ATOM | 7962 | N | VAL E 176 | 76.692 | 44.044 | 40.520 | 1.00 | 66.77 7 |
| | ATOM | 7963 | CA | VAL E 176 | 75.974 | 43.329 | 39.477 | 1.00 | 67.34 6 |
| | ATOM | 7964 | CB | VAL E 176 | 75.077 | 44.283 | 38.643 | 1.00 | 67.70 6 |
| 50 | ATOM | 7965 | CG1 | VAL E 176 | 74.430 | 43.524 | 37.479 | 1.00 | 66.11 6 |
| | ATOM | 7966 | CG2 | VAL E 176 | 74.009 | 44.902 | 39.537 | 1.00 | 66.22 6 |
| | ATOM | 7967 | C | VAL E 176 | 76.979 | 42.692 | 38.541 | 1.00 | 66.94 6 |
| | ATOM | 7968 | O | VAL E 176 | 77.894 | 43.354 | 38.078 | 1.00 | 65.94 8 |
| | ATOM | 7969 | N | THR E 177 | 76.796 | 41.407 | 38.265 | 1.00 | 68.37 7 |
| 55 | ATOM | 7970 | CA | THR E 177 | 77.682 | 40.671 | 37.362 | 1.00 | 70.46 6 |
| | ATOM | 7971 | CB | THR E 177 | 78.677 | 39.794 | 38.142 | 1.00 | 69.65 6 |
| | ATOM | 7972 | OG1 | THR E 177 | 77.962 | 38.938 | 39.041 | 1.00 | 68.82 8 |
| | ATOM | 7973 | CG2 | THR E 177 | 79.630 | 40.667 | 38.938 | 1.00 | 70.26 6 |
| | ATOM | 7974 | C | THR E 177 | 76.870 | 39.778 | 36.420 | 1.00 | 72.02 6 |
| 60 | ATOM | 7975 | O | THR E 177 | 75.849 | 39.202 | 36.813 | 1.00 | 72.47 8 |
| | ATOM | 7976 | N | GLN E 178 | 77.327 | 39.669 | 35.175 | 1.00 | 73.21 7 |
| | ATOM | 7977 | CA | GLN E 178 | 76.642 | 38.861 | 34.173 | 1.00 | 74.06 6 |
| | ATOM | 7978 | CB | GLN E 178 | 76.151 | 39.744 | 33.035 | 1.00 | 75.43 6 |
| | ATOM | 7979 | CG | GLN E 178 | 75.865 | 41.187 | 33.442 | 1.00 | 77.78 6 |
| | ATOM | 7980 | CD | GLN E 178 | 74.935 | 41.901 | 32.464 | 1.00 | 79.93 6 |

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|----|------|------|---------------|--------|--------|--------|------|-------|---|--|
| 5 | ATOM | 7981 | OE1 GLN E 178 | 75.139 | 41.862 | 31.236 | 1.00 | 82.06 | 8 | |
| | ATOM | 7982 | NE2 GLN E 178 | 73.909 | 42.565 | 33.002 | 1.00 | 78.21 | 7 | |
| | ATOM | 7983 | C GLN E 178 | 77.608 | 37.840 | 33.610 | 1.00 | 74.50 | 6 | |
| | ATOM | 7984 | O GLN E 178 | 78.661 | 38.205 | 33.086 | 1.00 | 74.89 | 8 | |
| | ATOM | 7985 | N LYS E 179 | 77.248 | 36.563 | 33.703 | 1.00 | 75.28 | 7 | |
| 10 | ATOM | 7986 | CA LYS E 179 | 78.107 | 35.482 | 33.209 | 1.00 | 75.34 | 6 | |
| | ATOM | 7987 | CB LYS E 179 | 78.666 | 34.692 | 34.391 | 1.00 | 77.30 | 6 | |
| | ATOM | 7988 | CG LYS E 179 | 79.186 | 35.600 | 35.515 | 1.00 | 81.23 | 6 | |
| | ATOM | 7989 | CD LYS E 179 | 79.593 | 34.805 | 36.763 | 1.00 | 83.79 | 6 | |
| | ATOM | 7990 | CE LYS E 179 | 79.779 | 35.727 | 37.981 | 1.00 | 82.73 | 6 | |
| 15 | ATOM | 7991 | NZ LYS E 179 | 78.496 | 36.431 | 38.332 | 1.00 | 82.45 | 7 | |
| | ATOM | 7992 | C LYS E 179 | 77.274 | 34.554 | 32.353 | 1.00 | 74.24 | 6 | |
| | ATOM | 7993 | O LYS E 179 | 76.409 | 33.850 | 32.882 | 1.00 | 74.20 | 8 | |
| | ATOM | 7994 | N LYS E 180 | 77.528 | 34.533 | 31.045 | 1.00 | 72.18 | 7 | |
| | ATOM | 7995 | CA LYS E 180 | 76.747 | 33.674 | 30.155 | 1.00 | 70.93 | 6 | |
| 20 | ATOM | 7996 | CB LYS E 180 | 77.062 | 34.017 | 28.694 | 1.00 | 71.21 | 6 | |
| | ATOM | 7997 | CG LYS E 180 | 78.412 | 33.558 | 28.187 | 1.00 | 67.95 | 6 | |
| | ATOM | 7998 | CD LYS E 180 | 78.327 | 32.136 | 27.630 | 1.00 | 67.85 | 6 | |
| | ATOM | 7999 | CE LYS E 180 | 77.429 | 32.041 | 26.394 | 1.00 | 66.39 | 6 | |
| | ATOM | 8000 | NZ LYS E 180 | 78.005 | 32.722 | 25.197 | 1.00 | 67.24 | 7 | |
| 25 | ATOM | 8001 | C LYS E 180 | 77.014 | 32.199 | 30.429 | 1.00 | 69.92 | 6 | |
| | ATOM | 8002 | O LYS E 180 | 77.803 | 31.876 | 31.303 | 1.00 | 70.33 | 8 | |
| | ATOM | 8003 | N ASN E 181 | 76.335 | 31.310 | 29.711 | 1.00 | 69.75 | 7 | |
| | ATOM | 8004 | CA ASN E 181 | 76.570 | 29.881 | 29.878 | 1.00 | 70.27 | 6 | |
| | ATOM | 8005 | CB ASN E 181 | 76.563 | 29.495 | 31.362 | 1.00 | 69.84 | 6 | |
| 30 | ATOM | 8006 | CG ASN E 181 | 75.395 | 30.060 | 32.112 | 1.00 | 70.39 | 6 | |
| | ATOM | 8007 | OD1 ASN E 181 | 74.255 | 30.006 | 31.648 | 1.00 | 75.03 | 8 | |
| | ATOM | 8008 | ND2 ASN E 181 | 75.659 | 30.587 | 33.299 | 1.00 | 70.26 | 7 | |
| | ATOM | 8009 | C ASN E 181 | 75.658 | 28.932 | 29.097 | 1.00 | 71.10 | 6 | |
| | ATOM | 8010 | O ASN E 181 | 74.438 | 28.918 | 29.276 | 1.00 | 72.53 | 8 | |
| 35 | ATOM | 8011 | N SER E 182 | 76.266 | 28.121 | 28.236 | 1.00 | 71.98 | 7 | |
| | ATOM | 8012 | CA SER E 182 | 75.518 | 27.161 | 27.427 | 1.00 | 73.38 | 6 | |
| | ATOM | 8013 | CB SER E 182 | 76.437 | 26.566 | 26.343 | 1.00 | 74.44 | 6 | |
| | ATOM | 8014 | OG SER E 182 | 75.712 | 25.791 | 25.388 | 1.00 | 77.56 | 8 | |
| | ATOM | 8015 | C SER E 182 | 74.984 | 26.054 | 28.345 | 1.00 | 73.19 | 6 | |
| 40 | ATOM | 8016 | O SER E 182 | 75.527 | 25.836 | 29.428 | 1.00 | 73.57 | 8 | |
| | ATOM | 8017 | N VAL E 183 | 73.936 | 25.350 | 27.914 | 1.00 | 72.44 | 7 | |
| | ATOM | 8018 | CA VAL E 183 | 73.341 | 24.295 | 28.738 | 1.00 | 71.01 | 6 | |
| | ATOM | 8019 | CB VAL E 183 | 72.582 | 24.906 | 29.956 | 1.00 | 69.59 | 6 | |
| | ATOM | 8020 | CG1 VAL E 183 | 71.892 | 26.184 | 29.555 | 1.00 | 67.54 | 6 | |
| 45 | ATOM | 8021 | CG2 VAL E 183 | 71.534 | 23.922 | 30.470 | 1.00 | 69.87 | 6 | |
| | ATOM | 8022 | C VAL E 183 | 72.366 | 23.391 | 27.986 | 1.00 | 71.36 | 6 | |
| | ATOM | 8023 | O VAL E 183 | 71.508 | 23.867 | 27.234 | 1.00 | 71.74 | 8 | |
| | ATOM | 8024 | N THR E 184 | 72.490 | 22.087 | 28.202 | 1.00 | 71.66 | 7 | |
| | ATOM | 8025 | CA THR E 184 | 71.586 | 21.134 | 27.551 | 1.00 | 73.71 | 6 | |
| 50 | ATOM | 8026 | CB THR E 184 | 72.339 | 19.902 | 26.988 | 1.00 | 72.73 | 6 | |
| | ATOM | 8027 | OG1 THR E 184 | 73.243 | 20.327 | 25.957 | 1.00 | 72.08 | 8 | |
| | ATOM | 8028 | CG2 THR E 184 | 71.353 | 18.897 | 26.392 | 1.00 | 71.99 | 6 | |
| | ATOM | 8029 | C THR E 184 | 70.547 | 20.656 | 28.565 | 1.00 | 75.19 | 6 | |
| | ATOM | 8030 | O THR E 184 | 70.862 | 20.458 | 29.740 | 1.00 | 75.50 | 8 | |
| 55 | ATOM | 8031 | N TYR E 185 | 69.307 | 20.495 | 28.110 | 1.00 | 76.63 | 7 | |
| | ATOM | 8032 | CA TYR E 185 | 68.234 | 20.054 | 28.992 | 1.00 | 77.67 | 6 | |
| | ATOM | 8033 | CB TYR E 185 | 67.084 | 21.074 | 29.004 | 1.00 | 78.57 | 6 | |
| | ATOM | 8034 | CG TYR E 185 | 67.547 | 22.482 | 29.285 | 1.00 | 78.26 | 6 | |
| | ATOM | 8035 | CD1 TYR E 185 | 68.203 | 23.218 | 28.304 | 1.00 | 77.24 | 6 | |
| 60 | ATOM | 8036 | CE1 TYR E 185 | 68.666 | 24.506 | 28.559 | 1.00 | 79.16 | 6 | |
| | ATOM | 8037 | CD2 TYR E 185 | 67.361 | 23.065 | 30.544 | 1.00 | 79.06 | 6 | |
| | ATOM | 8038 | CE2 TYR E 185 | 67.822 | 24.359 | 30.817 | 1.00 | 79.31 | 6 | |
| | ATOM | 8039 | CZ TYR E 185 | 68.472 | 25.075 | 29.819 | 1.00 | 79.42 | 6 | |
| | ATOM | 8040 | OH TYR E 185 | 68.919 | 26.357 | 30.067 | 1.00 | 80.13 | 8 | |
| | ATOM | 8041 | C TYR E 185 | 67.725 | 18.723 | 28.516 | 1.00 | 77.68 | 6 | |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|----|
| 5 | ATOM | 8042 | O | TYR E 185 | 67.578 | 18.509 | 27.314 | 1.00 | 76.95 | 8 |
| | ATOM | 8043 | N | SER E 186 | 67.460 | 17.831 | 29.463 | 1.00 | 79.15 | 7 |
| | ATOM | 8044 | CA | SER E 186 | 66.968 | 16.497 | 29.134 | 1.00 | 80.95 | 6 |
| | ATOM | 8045 | CB | SER E 186 | 66.593 | 15.755 | 30.423 | 1.00 | 81.59 | 6 |
| | ATOM | 8046 | OG | SER E 186 | 65.784 | 16.580 | 31.254 | 1.00 | 83.29 | 8 |
| 10 | ATOM | 8047 | C | SER E 186 | 65.770 | 16.594 | 28.192 | 1.00 | 81.27 | 6 |
| | ATOM | 8048 | O | SER E 186 | 65.612 | 15.764 | 27.291 | 1.00 | 81.31 | 8 |
| | ATOM | 8049 | N | CYS E 187 | 64.948 | 17.624 | 28.402 | 1.00 | 82.15 | 7 |
| | ATOM | 8050 | CA | CYS E 187 | 63.753 | 17.876 | 27.583 | 1.00 | 83.38 | 6 |
| | ATOM | 8051 | C | CYS E 187 | 64.119 | 18.104 | 26.143 | 1.00 | 83.62 | 6 |
| 15 | ATOM | 8052 | O | CYS E 187 | 63.463 | 17.631 | 25.206 | 1.00 | 82.88 | 8 |
| | ATOM | 8053 | CB | CYS E 187 | 63.043 | 19.179 | 27.993 | 1.00 | 83.49 | 6 |
| | ATOM | 8054 | SG | CYS E 187 | 63.980 | 20.757 | 27.703 | 1.00 | 86.50 | 16 |
| | ATOM | 8055 | N | CYS E 188 | 65.204 | 18.841 | 25.993 | 1.00 | 84.35 | 7 |
| | ATOM | 8056 | CA | CYS E 188 | 65.589 | 19.318 | 24.701 | 1.00 | 84.60 | 6 |
| 20 | ATOM | 8057 | C | CYS E 188 | 67.013 | 18.991 | 24.213 | 1.00 | 84.20 | 6 |
| | ATOM | 8058 | O | CYS E 188 | 68.012 | 19.334 | 24.874 | 1.00 | 84.71 | 8 |
| | ATOM | 8059 | CB | CYS E 188 | 65.319 | 20.833 | 24.759 | 1.00 | 85.11 | 6 |
| | ATOM | 8060 | SG | CYS E 188 | 63.808 | 21.349 | 25.731 | 1.00 | 88.15 | 16 |
| | ATOM | 8061 | N | PRO E 189 | 67.108 | 18.340 | 23.025 | 1.00 | 83.48 | 7 |
| 25 | ATOM | 8062 | CD | PRO E 189 | 65.864 | 18.064 | 22.267 | 1.00 | 82.84 | 6 |
| | ATOM | 8063 | CA | PRO E 189 | 68.292 | 17.878 | 22.267 | 1.00 | 81.51 | 6 |
| | ATOM | 8064 | CB | PRO E 189 | 67.738 | 17.666 | 20.853 | 1.00 | 82.30 | 6 |
| | ATOM | 8065 | CG | PRO E 189 | 66.345 | 17.173 | 21.119 | 1.00 | 82.79 | 6 |
| | ATOM | 8066 | C | PRO E 189 | 69.547 | 18.782 | 22.249 | 1.00 | 79.46 | 6 |
| 30 | ATOM | 8067 | O | PRO E 189 | 70.592 | 18.398 | 22.785 | 1.00 | 79.36 | 8 |
| | ATOM | 8068 | N | GLU E 190 | 69.450 | 19.961 | 21.629 | 1.00 | 76.55 | 7 |
| | ATOM | 8069 | CA | GLU E 190 | 70.592 | 20.878 | 21.529 | 1.00 | 74.34 | 6 |
| | ATOM | 8070 | CB | GLU E 190 | 70.358 | 21.881 | 20.401 | 1.00 | 76.82 | 6 |
| | ATOM | 8071 | CG | GLU E 190 | 69.520 | 21.352 | 19.239 | 1.00 | 80.12 | 6 |
| 35 | ATOM | 8072 | CD | GLU E 190 | 70.336 | 20.533 | 18.231 | 1.00 | 81.75 | 6 |
| | ATOM | 8073 | OE1 | GLU E 190 | 71.471 | 20.965 | 17.884 | 1.00 | 81.85 | 8 |
| | ATOM | 8074 | OE2 | GLU E 190 | 69.836 | 19.472 | 17.775 | 1.00 | 80.52 | 8 |
| | ATOM | 8075 | C | GLU E 190 | 70.822 | 21.663 | 22.815 | 1.00 | 71.33 | 6 |
| | ATOM | 8076 | O | GLU E 190 | 70.095 | 21.489 | 23.791 | 1.00 | 71.05 | 8 |
| 40 | ATOM | 8077 | N | ALA E 191 | 71.826 | 22.543 | 22.798 | 1.00 | 68.78 | 7 |
| | ATOM | 8078 | CA | ALA E 191 | 72.142 | 23.390 | 23.957 | 1.00 | 67.15 | 6 |
| | ATOM | 8079 | CB | ALA E 191 | 73.651 | 23.536 | 24.108 | 1.00 | 65.15 | 6 |
| | ATOM | 8080 | C | ALA E 191 | 71.502 | 24.787 | 23.836 | 1.00 | 65.83 | 6 |
| | ATOM | 8081 | O | ALA E 191 | 71.379 | 25.340 | 22.730 | 1.00 | 64.00 | 8 |
| 45 | ATOM | 8082 | N | TYR E 192 | 71.097 | 25.355 | 24.971 | 1.00 | 64.83 | 7 |
| | ATOM | 8083 | CA | TYR E 192 | 70.487 | 26.678 | 24.964 | 1.00 | 65.12 | 6 |
| | ATOM | 8084 | CB | TYR E 192 | 69.025 | 26.613 | 25.450 | 1.00 | 63.81 | 6 |
| | ATOM | 8085 | CG | TYR E 192 | 68.096 | 25.953 | 24.462 | 1.00 | 63.14 | 6 |
| | ATOM | 8086 | CD1 | TYR E 192 | 67.939 | 24.564 | 24.442 | 1.00 | 64.40 | 6 |
| 50 | ATOM | 8087 | CE1 | TYR E 192 | 67.146 | 23.934 | 23.468 | 1.00 | 64.53 | 6 |
| | ATOM | 8088 | CD2 | TYR E 192 | 67.435 | 26.705 | 23.493 | 1.00 | 62.60 | 6 |
| | ATOM | 8089 | CE2 | TYR E 192 | 66.642 | 26.094 | 22.521 | 1.00 | 64.04 | 6 |
| | ATOM | 8090 | CZ | TYR E 192 | 66.505 | 24.710 | 22.512 | 1.00 | 64.71 | 6 |
| | ATOM | 8091 | OH | TYR E 192 | 65.744 | 24.101 | 21.538 | 1.00 | 66.46 | 8 |
| 55 | ATOM | 8092 | C | TYR E 192 | 71.262 | 27.694 | 25.795 | 1.00 | 65.22 | 6 |
| | ATOM | 8093 | O | TYR E 192 | 71.181 | 27.699 | 27.026 | 1.00 | 67.13 | 8 |
| | ATOM | 8094 | N | GLU E 193 | 72.010 | 28.557 | 25.112 | 1.00 | 65.61 | 7 |
| | ATOM | 8095 | CA | GLU E 193 | 72.792 | 29.606 | 25.773 | 1.00 | 64.70 | 6 |
| | ATOM | 8096 | CB | GLU E 193 | 73.643 | 30.372 | 24.749 | 1.00 | 66.19 | 6 |
| 60 | ATOM | 8097 | CG | GLU E 193 | 74.722 | 29.522 | 24.074 | 1.00 | 69.50 | 6 |
| | ATOM | 8098 | CD | GLU E 193 | 75.625 | 30.345 | 23.144 | 1.00 | 72.29 | 6 |
| | ATOM | 8099 | OE1 | GLU E 193 | 76.083 | 31.435 | 23.584 | 1.00 | 71.70 | 8 |
| | ATOM | 8100 | OE2 | GLU E 193 | 75.881 | 29.898 | 21.985 | 1.00 | 73.48 | 8 |
| | ATOM | 8101 | C | GLU E 193 | 71.890 | 30.600 | 26.498 | 1.00 | 63.08 | 6 |
| | ATOM | 8102 | O | GLU E 193 | 70.747 | 30.828 | 26.095 | 1.00 | 64.03 | 8 |

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|----|------|------|-----|-----------|--------|--------|--------|------|-------|---|--|--|--|--|
| 5 | ATOM | 8103 | N | ASP E 194 | 72.418 | 31.187 | 27.566 | 1.00 | 62.00 | 7 | | | | |
| | ATOM | 8104 | CA | ASP E 194 | 71.683 | 32.168 | 28.340 | 1.00 | 60.31 | 6 | | | | |
| | ATOM | 8105 | CB | ASP E 194 | 70.644 | 31.480 | 29.235 | 1.00 | 62.01 | 6 | | | | |
| | ATOM | 8106 | CG | ASP E 194 | 71.268 | 30.749 | 30.413 | 1.00 | 64.58 | 6 | | | | |
| | ATOM | 8107 | OD1 | ASP E 194 | 71.200 | 29.504 | 30.448 | 1.00 | 66.44 | 8 | | | | |
| 10 | ATOM | 8108 | OD2 | ASP E 194 | 71.824 | 31.415 | 31.314 | 1.00 | 64.95 | 8 | | | | |
| | ATOM | 8109 | C | ASP E 194 | 72.637 | 32.989 | 29.193 | 1.00 | 59.18 | 6 | | | | |
| | ATOM | 8110 | O | ASP E 194 | 73.715 | 32.515 | 29.570 | 1.00 | 59.24 | 8 | | | | |
| | ATOM | 8111 | N | VAL E 195 | 72.238 | 34.223 | 29.484 | 1.00 | 56.73 | 7 | | | | |
| | ATOM | 8112 | CA | VAL E 195 | 73.029 | 35.121 | 30.311 | 1.00 | 55.51 | 6 | | | | |
| 15 | ATOM | 8113 | CB | VAL E 195 | 73.019 | 36.555 | 29.763 | 1.00 | 53.92 | 6 | | | | |
| | ATOM | 8114 | CG1 | VAL E 195 | 73.686 | 37.498 | 30.752 | 1.00 | 53.41 | 6 | | | | |
| | ATOM | 8115 | CG2 | VAL E 195 | 73.738 | 36.595 | 28.431 | 1.00 | 55.34 | 6 | | | | |
| | ATOM | 8116 | C | VAL E 195 | 72.453 | 35.145 | 31.715 | 1.00 | 56.03 | 6 | | | | |
| | ATOM | 8117 | O | VAL E 195 | 71.270 | 35.400 | 31.907 | 1.00 | 56.70 | 8 | | | | |
| 20 | ATOM | 8118 | N | GLU E 196 | 73.292 | 34.868 | 32.702 | 1.00 | 57.06 | 7 | | | | |
| | ATOM | 8119 | CA | GLU E 196 | 72.834 | 34.870 | 34.077 | 1.00 | 57.01 | 6 | | | | |
| | ATOM | 8120 | CB | GLU E 196 | 73.402 | 33.673 | 34.821 | 1.00 | 57.41 | 6 | | | | |
| | ATOM | 8121 | CG | GLU E 196 | 72.908 | 33.555 | 36.238 | 1.00 | 61.42 | 6 | | | | |
| | ATOM | 8122 | CD | GLU E 196 | 73.533 | 32.383 | 36.968 | 1.00 | 62.69 | 6 | | | | |
| 25 | ATOM | 8123 | OE1 | GLU E 196 | 73.377 | 31.235 | 36.493 | 1.00 | 64.88 | 8 | | | | |
| | ATOM | 8124 | OE2 | GLU E 196 | 74.184 | 32.604 | 38.013 | 1.00 | 64.76 | 8 | | | | |
| | ATOM | 8125 | C | GLU E 196 | 73.315 | 36.160 | 34.715 | 1.00 | 57.51 | 6 | | | | |
| | ATOM | 8126 | O | GLU E 196 | 74.518 | 36.427 | 34.755 | 1.00 | 60.16 | 8 | | | | |
| | ATOM | 8127 | N | VAL E 197 | 72.375 | 36.969 | 35.192 | 1.00 | 55.54 | 7 | | | | |
| 30 | ATOM | 8128 | CA | VAL E 197 | 72.712 | 38.226 | 35.829 | 1.00 | 54.09 | 6 | | | | |
| | ATOM | 8129 | CB | VAL E 197 | 71.853 | 39.380 | 35.278 | 1.00 | 50.90 | 6 | | | | |
| | ATOM | 8130 | CG1 | VAL E 197 | 72.241 | 40.685 | 35.932 | 1.00 | 47.64 | 6 | | | | |
| | ATOM | 8131 | CG2 | VAL E 197 | 72.030 | 39.471 | 33.782 | 1.00 | 49.59 | 6 | | | | |
| | ATOM | 8132 | C | VAL E 197 | 72.473 | 38.067 | 37.325 | 1.00 | 56.97 | 6 | | | | |
| 35 | ATOM | 8133 | O | VAL E 197 | 71.414 | 37.614 | 37.748 | 1.00 | 58.03 | 8 | | | | |
| | ATOM | 8134 | N | SER E 198 | 73.476 | 38.409 | 38.125 | 1.00 | 58.05 | 7 | | | | |
| | ATOM | 8135 | CA | SER E 198 | 73.338 | 38.300 | 39.562 | 1.00 | 58.55 | 6 | | | | |
| | ATOM | 8136 | CB | SER E 198 | 74.550 | 37.584 | 40.174 | 1.00 | 58.65 | 6 | | | | |
| | ATOM | 8137 | OG | SER E 198 | 74.556 | 36.209 | 39.811 | 1.00 | 60.87 | 8 | | | | |
| 40 | ATOM | 8138 | C | SER E 198 | 73.182 | 39.685 | 40.155 | 1.00 | 58.53 | 6 | | | | |
| | ATOM | 8139 | O | SER E 198 | 74.049 | 40.549 | 40.004 | 1.00 | 59.57 | 8 | | | | |
| | ATOM | 8140 | N | LEU E 199 | 72.060 | 39.895 | 40.823 | 1.00 | 58.51 | 7 | | | | |
| | ATOM | 8141 | CA | LEU E 199 | 71.803 | 41.176 | 41.434 | 1.00 | 59.74 | 6 | | | | |
| | ATOM | 8142 | CB | LEU E 199 | 70.361 | 41.612 | 41.186 | 1.00 | 59.28 | 6 | | | | |
| 45 | ATOM | 8143 | CG | LEU E 199 | 69.921 | 42.861 | 41.953 | 1.00 | 58.45 | 6 | | | | |
| | ATOM | 8144 | CD1 | LEU E 199 | 70.758 | 44.059 | 41.543 | 1.00 | 57.64 | 6 | | | | |
| | ATOM | 8145 | CD2 | LEU E 199 | 68.466 | 43.127 | 41.669 | 1.00 | 57.53 | 6 | | | | |
| | ATOM | 8146 | C | LEU E 199 | 72.039 | 41.084 | 42.917 | 1.00 | 61.63 | 6 | | | | |
| | ATOM | 8147 | O | LEU E 199 | 71.226 | 40.500 | 43.640 | 1.00 | 64.16 | 8 | | | | |
| 50 | ATOM | 8148 | N | ASN E 200 | 73.163 | 41.637 | 43.366 | 1.00 | 61.69 | 7 | | | | |
| | ATOM | 8149 | CA | ASN E 200 | 73.486 | 41.658 | 44.780 | 1.00 | 58.91 | 6 | | | | |
| | ATOM | 8150 | CB | ASN E 200 | 74.981 | 41.477 | 44.994 | 1.00 | 61.22 | 6 | | | | |
| | ATOM | 8151 | CG | ASN E 200 | 75.355 | 41.522 | 46.454 | 1.00 | 63.36 | 6 | | | | |
| | ATOM | 8152 | OD1 | ASN E 200 | 74.686 | 40.916 | 47.295 | 1.00 | 64.82 | 8 | | | | |
| 55 | ATOM | 8153 | ND2 | ASN E 200 | 76.426 | 42.235 | 46.770 | 1.00 | 64.37 | 7 | | | | |
| | ATOM | 8154 | C | ASN E 200 | 73.048 | 43.026 | 45.280 | 1.00 | 56.95 | 6 | | | | |
| | ATOM | 8155 | O | ASN E 200 | 73.610 | 44.056 | 44.905 | 1.00 | 58.64 | 8 | | | | |
| | ATOM | 8156 | N | PHE E 201 | 72.018 | 43.030 | 46.109 | 1.00 | 54.18 | 7 | | | | |
| | ATOM | 8157 | CA | PHE E 201 | 71.474 | 44.260 | 46.650 | 1.00 | 52.16 | 6 | | | | |
| 60 | ATOM | 8158 | CB | PHE E 201 | 70.257 | 44.688 | 45.844 | 1.00 | 50.83 | 6 | | | | |
| | ATOM | 8159 | CG | PHE E 201 | 69.065 | 43.780 | 46.028 | 1.00 | 47.47 | 6 | | | | |
| | ATOM | 8160 | CD1 | PHE E 201 | 67.923 | 44.233 | 46.681 | 1.00 | 47.04 | 6 | | | | |
| | ATOM | 8161 | CD2 | PHE E 201 | 69.107 | 42.458 | 45.601 | 1.00 | 44.93 | 6 | | | | |
| | ATOM | 8162 | CE1 | PHE E 201 | 66.843 | 43.382 | 46.911 | 1.00 | 45.49 | 6 | | | | |
| | ATOM | 8163 | CE2 | PHE E 201 | 68.043 | 41.608 | 45.829 | 1.00 | 43.88 | 6 | | | | |

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|----|------|------|------|-----------|--------|--------|--------|------|-------|----|--|
| 5 | ATOM | 8164 | CZ | PHE E 201 | 66.905 | 42.072 | 46.488 | 1.00 | 43.86 | 6 | |
| | ATOM | 8165 | C | PHE E 201 | 71.029 | 43.977 | 48.066 | 1.00 | 53.50 | 6 | |
| | ATOM | 8166 | O | PHE E 201 | 71.001 | 42.823 | 48.504 | 1.00 | 53.30 | 8 | |
| | ATOM | 8167 | N | ARG E 202 | 70.650 | 45.032 | 48.770 | 1.00 | 55.04 | 7 | |
| | ATOM | 8168 | CA | ARG E 202 | 70.195 | 44.915 | 50.146 | 1.00 | 57.24 | 6 | |
| 10 | ATOM | 8169 | CB | ARG E 202 | 71.399 | 44.898 | 51.084 | 1.00 | 59.58 | 6 | |
| | ATOM | 8170 | CG | ARG E 202 | 72.078 | 46.254 | 51.130 | 1.00 | 64.26 | 6 | |
| | ATOM | 8171 | CD | ARG E 202 | 73.337 | 46.278 | 51.951 | 1.00 | 65.59 | 6 | |
| | ATOM | 8172 | NE | ARG E 202 | 73.935 | 47.606 | 51.908 | 1.00 | 67.13 | 7 | |
| | ATOM | 8173 | CZ | ARG E 202 | 75.140 | 47.891 | 52.386 | 1.00 | 68.53 | 6 | |
| 15 | ATOM | 8174 | NH1 | ARG E 202 | 75.870 | 46.930 | 52.942 | 1.00 | 69.03 | 7 | |
| | ATOM | 8175 | NH2 | ARG E 202 | 75.612 | 49.129 | 52.303 | 1.00 | 68.11 | 7 | |
| | ATOM | 8176 | C | ARG E 202 | 69.321 | 46.121 | 50.499 | 1.00 | 57.27 | 6 | |
| | ATOM | 8177 | O | ARG E 202 | 69.370 | 47.167 | 49.839 | 1.00 | 56.88 | 8 | |
| | ATOM | 8178 | N | LYS E 203 | 68.528 | 45.974 | 51.551 | 1.00 | 56.76 | 7 | |
| 20 | ATOM | 8179 | CA | LYS E 203 | 67.689 | 47.063 | 52.011 | 1.00 | 57.10 | 6 | |
| | ATOM | 8180 | CB | LYS E 203 | 66.755 | 46.583 | 53.109 | 1.00 | 58.42 | 6 | |
| | ATOM | 8181 | CG | LYS E 203 | 65.904 | 47.682 | 53.702 | 1.00 | 60.29 | 6 | |
| | ATOM | 8182 | CD | LYS E 203 | 65.112 | 47.157 | 54.883 | 1.00 | 64.62 | 6 | |
| | ATOM | 8183 | CE | LYS E 203 | 64.222 | 48.241 | 55.471 | 1.00 | 67.46 | 6 | |
| 25 | ATOM | 8184 | NZ | LYS E 203 | 63.171 | 48.696 | 54.504 | 1.00 | 70.79 | 7 | |
| | ATOM | 8185 | C | LYS E 203 | 68.623 | 48.101 | 52.603 | 1.00 | 56.53 | 6 | |
| | ATOM | 8186 | O | LYS E 203 | 69.715 | 47.769 | 53.060 | 1.00 | 58.18 | 8 | |
| | ATOM | 8187 | N | LYS E 204 | 68.190 | 49.352 | 52.629 | 1.00 | 53.82 | 7 | |
| | ATOM | 8188 | CA | LYS E 204 | 69.021 | 50.392 | 53.207 | 1.00 | 52.45 | 6 | |
| 30 | ATOM | 8189 | CB | LYS E 204 | 68.545 | 51.766 | 52.731 | 1.00 | 50.86 | 6 | |
| | ATOM | 8190 | CG | LYS E 204 | 68.852 | 52.110 | 51.279 | 1.00 | 44.94 | 6 | |
| | ATOM | 8191 | CD | LYS E 204 | 68.253 | 53.462 | 50.970 | 1.00 | 45.54 | 6 | |
| | ATOM | 8192 | CE | LYS E 204 | 68.744 | 54.050 | 49.669 | 1.00 | 46.91 | 6 | |
| | ATOM | 8193 | NZ | LYS E 204 | 68.388 | 53.268 | 48.463 | 1.00 | 48.94 | 7 | |
| 35 | ATOM | 8194 | C | LYS E 204 | 68.991 | 50.317 | 54.747 | 1.00 | 54.01 | 6 | |
| | ATOM | 8195 | O | LYS E 204 | 68.119 | 49.668 | 55.329 | 1.00 | 54.82 | 8 | |
| | ATOM | 8196 | N | GLY E 205 | 69.958 | 50.969 | 55.394 | 1.00 | 53.51 | 7 | |
| | ATOM | 8197 | CA | GLY E 205 | 70.025 | 50.987 | 56.848 | 1.00 | 52.96 | 6 | |
| | ATOM | 8198 | C | GLY E 205 | 69.747 | 52.400 | 57.344 | 1.00 | 54.24 | 6 | |
| 40 | ATOM | 8199 | OT1 | GLY E 205 | 69.326 | 53.224 | 56.507 | 1.00 | 53.02 | 8 | |
| | ATOM | 8200 | OT2 | GLY E 205 | 69.937 | 52.697 | 58.551 | 1.00 | 54.73 | 8 | |
| | ATOM | 8201 | OH2 | WAT W 1 | 42.707 | 26.844 | 16.535 | 1.00 | 50.04 | 8 | |
| | ATOM | 8202 | OH2 | WAT W 2 | 46.115 | 22.922 | 8.819 | 1.00 | 33.72 | 8 | |
| | ATOM | 8203 | OH2 | WAT W 3 | 49.921 | 22.962 | 13.240 | 1.00 | 27.71 | 8 | |
| 45 | ATOM | 8204 | OH2 | WAT W 4 | 48.219 | 24.526 | 9.434 | 1.00 | 48.75 | 8 | |
| | ATOM | 8205 | OH2 | WAT W 5 | 27.826 | 41.690 | 17.095 | 1.00 | 41.54 | 8 | |
| | ATOM | 8206 | OH2 | WAT W 6 | 24.872 | 36.589 | 8.613 | 1.00 | 51.20 | 8 | |
| | ATOM | 8207 | OH2 | WAT W 7 | 36.046 | 60.034 | 17.934 | 1.00 | 33.21 | 8 | |
| | ATOM | 8208 | OH2 | WAT W 8 | 35.043 | 57.811 | 16.418 | 1.00 | 28.29 | 8 | |
| 50 | ATOM | 8209 | OH2 | WAT W 9 | 55.882 | 56.455 | 16.997 | 1.00 | 31.72 | 8 | |
| | ATOM | 8210 | OH2 | WAT W 10 | 55.717 | 62.292 | 9.132 | 1.00 | 41.99 | 8 | |
| | ATOM | 8211 | OH2 | WAT W 11 | 54.077 | 57.638 | 15.628 | 1.00 | 35.89 | 8 | |
| | ATOM | 8212 | OH2 | WAT W 12 | 60.807 | 36.700 | 17.893 | 1.00 | 31.22 | 8 | |
| | ATOM | 8213 | OH2 | WAT W 13 | 66.541 | 42.748 | 13.082 | 1.00 | 52.94 | 8 | |
| 55 | ATOM | 8214 | OH2 | WAT W 14 | 64.752 | 41.327 | 9.587 | 1.00 | 53.75 | 8 | |
| | ATOM | 8215 | CA+2 | CA2 I 1 | 56.450 | 11.097 | 37.999 | 1.00 | 76.79 | 20 | |
| | ATOM | 8216 | CL-1 | CL1 I 2 | 37.092 | 21.684 | 12.754 | 1.00 | 43.91 | 17 | |
| | ATOM | 8217 | CA+2 | CA2 I 3 | 17.667 | 23.110 | 38.506 | 1.00 | 80.38 | 20 | |
| | ATOM | 8218 | CL-1 | CL1 I 4 | 20.502 | 44.774 | 13.190 | 1.00 | 62.37 | 17 | |
| 60 | ATOM | 8219 | CA+2 | CA2 I 5 | 16.762 | 64.154 | 38.299 | 1.00 | 85.82 | 20 | |
| | ATOM | 8220 | CL-1 | CL1 I 6 | 37.412 | 67.363 | 13.067 | 1.00 | 45.17 | 17 | |
| | ATOM | 8221 | CA+2 | CA2 I 7 | 55.038 | 76.858 | 37.301 | 1.00 | 71.00 | 20 | |
| | ATOM | 8222 | CL-1 | CL1 I 8 | 64.026 | 57.746 | 12.334 | 1.00 | 69.47 | 17 | |
| | ATOM | 8223 | CA+2 | CA2 I 9 | 79.499 | 45.067 | 37.836 | 1.00 | 85.28 | 20 | |
| | ATOM | 8224 | CL-1 | CL1 I 10 | 64.286 | 29.844 | 12.440 | 1.00 | 48.05 | 17 | |

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|----|------|------|----|-------|---|--------|--------|--------|------------|----|
| 5 | ATOM | 8225 | C1 | HEP L | 1 | 31.694 | 22.169 | 23.679 | 1.00109.78 | 6 |
| | ATOM | 8226 | C2 | HEP L | 1 | 32.042 | 22.822 | 25.000 | 1.00106.01 | 6 |
| | ATOM | 8227 | C3 | HEP L | 1 | 33.258 | 20.667 | 25.468 | 1.00 99.68 | 6 |
| | ATOM | 8228 | C4 | HEP L | 1 | 34.107 | 19.901 | 26.462 | 1.00 97.90 | 6 |
| | ATOM | 8229 | C5 | HEP L | 1 | 33.049 | 21.220 | 28.203 | 1.00 99.77 | 6 |
| | ATOM | 8230 | C6 | HEP L | 1 | 32.154 | 21.953 | 27.266 | 1.00101.85 | 6 |
| | ATOM | 8231 | C7 | HEP L | 1 | 34.051 | 19.067 | 28.833 | 1.00 98.50 | 6 |
| | ATOM | 8232 | C8 | HEP L | 1 | 35.030 | 19.802 | 29.773 | 1.00 97.76 | 6 |
| 10 | ATOM | 8233 | O4 | HEP L | 1 | 34.441 | 19.860 | 31.064 | 1.00 96.20 | 8 |
| | ATOM | 8234 | N1 | HEP L | 1 | 32.880 | 22.043 | 25.968 | 1.00103.11 | 7 |
| | ATOM | 8235 | S1 | HEP L | 1 | 31.207 | 23.336 | 22.418 | 1.00113.66 | 16 |
| | ATOM | 8236 | O1 | HEP L | 1 | 31.826 | 22.878 | 21.182 | 1.00113.59 | 8 |
| 15 | ATOM | 8237 | O2 | HEP L | 1 | 31.477 | 24.685 | 22.941 | 1.00111.64 | 8 |
| | ATOM | 8238 | O3 | HEP L | 1 | 29.701 | 23.322 | 22.307 | 1.00111.51 | 8 |
| | ATOM | 8239 | N2 | HEP L | 1 | 33.333 | 19.839 | 27.737 | 1.00 98.16 | 7 |
| | ATOM | 8240 | C1 | HEP L | 2 | 19.833 | 49.708 | 24.248 | 1.00108.88 | 6 |
| | ATOM | 8241 | C2 | HEP L | 2 | 20.653 | 49.684 | 25.518 | 1.00104.63 | 6 |
| | ATOM | 8242 | C3 | HEP L | 2 | 19.090 | 47.814 | 26.172 | 1.00100.27 | 6 |
| 20 | ATOM | 8243 | C4 | HEP L | 2 | 18.728 | 46.788 | 27.241 | 1.00 98.30 | 6 |
| | ATOM | 8244 | C5 | HEP L | 2 | 19.702 | 48.326 | 28.859 | 1.00100.12 | 6 |
| | ATOM | 8245 | C6 | HEP L | 2 | 20.022 | 49.380 | 27.845 | 1.00101.78 | 6 |
| | ATOM | 8246 | C7 | HEP L | 2 | 18.080 | 46.646 | 29.663 | 1.00 97.02 | 6 |
| | ATOM | 8247 | C8 | HEP L | 2 | 19.186 | 46.065 | 30.550 | 1.00 96.36 | 6 |
| | ATOM | 8248 | O4 | HEP L | 2 | 19.161 | 46.714 | 31.805 | 1.00 95.77 | 8 |
| 25 | ATOM | 8249 | N1 | HEP L | 2 | 20.281 | 48.676 | 26.560 | 1.00102.78 | 7 |
| | ATOM | 8250 | S1 | HEP L | 2 | 20.640 | 50.530 | 22.892 | 1.00112.59 | 16 |
| | ATOM | 8251 | O1 | HEP L | 2 | 20.348 | 49.765 | 21.697 | 1.00113.24 | 8 |
| | ATOM | 8252 | O2 | HEP L | 2 | 22.024 | 50.791 | 23.309 | 1.00111.25 | 8 |
| 30 | ATOM | 8253 | O3 | HEP L | 2 | 20.059 | 51.924 | 22.770 | 1.00111.32 | 8 |
| | ATOM | 8254 | N2 | HEP L | 2 | 18.478 | 47.544 | 28.507 | 1.00 98.39 | 7 |
| | ATOM | 8255 | C1 | HEP L | 3 | 42.028 | 70.369 | 23.900 | 1.00109.55 | 6 |
| | ATOM | 8256 | C2 | HEP L | 3 | 42.091 | 69.312 | 25.003 | 1.00104.54 | 6 |
| | ATOM | 8257 | C3 | HEP L | 3 | 40.178 | 70.594 | 25.988 | 1.00 97.17 | 6 |
| | ATOM | 8258 | C4 | HEP L | 3 | 39.192 | 70.688 | 27.124 | 1.00 96.78 | 6 |
| 35 | ATOM | 8259 | C5 | HEP L | 3 | 40.844 | 69.540 | 28.502 | 1.00 98.62 | 6 |
| | ATOM | 8260 | C6 | HEP L | 3 | 41.854 | 69.476 | 27.408 | 1.00100.28 | 6 |
| | ATOM | 8261 | C7 | HEP L | 3 | 39.103 | 70.891 | 29.639 | 1.00 97.37 | 6 |
| | ATOM | 8262 | C8 | HEP L | 3 | 38.600 | 69.616 | 30.336 | 1.00 97.34 | 6 |
| 40 | ATOM | 8263 | O4 | HEP L | 3 | 39.310 | 69.466 | 31.552 | 1.00 95.42 | 8 |
| | ATOM | 8264 | N1 | HEP L | 3 | 41.104 | 69.418 | 26.123 | 1.00100.25 | 7 |
| | ATOM | 8265 | S1 | HEP L | 3 | 42.851 | 69.897 | 22.390 | 1.00113.40 | 16 |
| | ATOM | 8266 | O1 | HEP L | 3 | 41.999 | 70.352 | 21.301 | 1.00112.83 | 8 |
| | ATOM | 8267 | O2 | HEP L | 3 | 43.216 | 68.464 | 22.535 | 1.00111.97 | 8 |
| | ATOM | 8268 | O3 | HEP L | 3 | 44.208 | 70.580 | 22.342 | 1.00111.22 | 8 |
| 45 | ATOM | 8269 | N2 | HEP L | 3 | 39.982 | 70.756 | 28.394 | 1.00 97.91 | 7 |
| | ATOM | 8270 | C1 | HEP L | 4 | 67.843 | 54.529 | 23.109 | 1.00109.23 | 6 |
| | ATOM | 8271 | C2 | HEP L | 4 | 67.696 | 54.053 | 24.549 | 1.00105.70 | 6 |
| | ATOM | 8272 | C3 | HEP L | 4 | 67.448 | 56.488 | 25.071 | 1.00101.29 | 6 |
| 50 | ATOM | 8273 | C4 | HEP L | 4 | 67.199 | 57.526 | 26.150 | 1.00 99.73 | 6 |
| | ATOM | 8274 | C5 | HEP L | 4 | 68.223 | 55.960 | 27.701 | 1.00100.32 | 6 |
| | ATOM | 8275 | C6 | HEP L | 4 | 68.526 | 54.948 | 26.646 | 1.00101.68 | 6 |
| | ATOM | 8276 | C7 | HEP L | 4 | 68.126 | 58.362 | 28.296 | 1.00 99.92 | 6 |
| | ATOM | 8277 | C8 | HEP L | 4 | 67.284 | 58.007 | 29.528 | 1.00100.01 | 6 |
| | ATOM | 8278 | O4 | HEP L | 4 | 68.179 | 57.751 | 30.594 | 1.00100.41 | 8 |
| 55 | ATOM | 8279 | N1 | HEP L | 4 | 67.472 | 55.082 | 25.609 | 1.00103.08 | 7 |
| | ATOM | 8280 | S1 | HEP L | 4 | 67.556 | 53.252 | 21.895 | 1.00112.53 | 16 |
| | ATOM | 8281 | O1 | HEP L | 4 | 66.829 | 53.860 | 20.813 | 1.00112.71 | 8 |
| | ATOM | 8282 | O2 | HEP L | 4 | 67.011 | 52.080 | 22.599 | 1.00111.24 | 8 |
| 60 | ATOM | 8283 | O3 | HEP L | 4 | 68.908 | 52.765 | 21.423 | 1.00111.51 | 8 |
| | ATOM | 8284 | N2 | HEP L | 4 | 68.258 | 57.354 | 27.169 | 1.00 99.66 | 7 |
| | ATOM | 8285 | C1 | HEP L | 5 | 62.836 | 24.327 | 23.511 | 1.00108.64 | 6 |

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|----|------|------|----|-------|---|--------|--------|--------|------------|----|
| 5 | ATOM | 8286 | C2 | HEP L | 5 | 62.164 | 25.268 | 24.495 | 1.00104.37 | 6 |
| | ATOM | 8287 | C3 | HEP L | 5 | 64.426 | 25.352 | 25.555 | 1.00 99.26 | 6 |
| | ATOM | 8288 | C4 | HEP L | 5 | 65.270 | 25.934 | 26.676 | 1.00 98.50 | 6 |
| | ATOM | 8289 | C5 | HEP L | 5 | 63.215 | 26.126 | 27.960 | 1.00 99.10 | 6 |
| | ATOM | 8290 | C6 | HEP L | 5 | 62.366 | 25.505 | 26.903 | 1.00100.20 | 6 |
| 10 | ATOM | 8291 | C7 | HEP L | 5 | 65.381 | 26.089 | 29.165 | 1.00 98.56 | 6 |
| | ATOM | 8292 | C8 | HEP L | 5 | 65.085 | 27.500 | 29.708 | 1.00 98.97 | 6 |
| | ATOM | 8293 | O4 | HEP L | 5 | 64.379 | 27.406 | 30.942 | 1.00 98.36 | 8 |
| | ATOM | 8294 | N1 | HEP L | 5 | 63.001 | 25.830 | 25.594 | 1.00101.58 | 7 |
| | ATOM | 8295 | S1 | HEP L | 5 | 61.935 | 24.146 | 21.985 | 1.00112.71 | 16 |
| 15 | ATOM | 8296 | O1 | HEP L | 5 | 62.912 | 24.120 | 20.912 | 1.00112.36 | 8 |
| | ATOM | 8297 | O2 | HEP L | 5 | 60.852 | 25.151 | 22.006 | 1.00111.63 | 8 |
| | ATOM | 8298 | O3 | HEP L | 5 | 61.166 | 22.846 | 22.024 | 1.00111.95 | 8 |
| | ATOM | 8299 | N2 | HEP L | 5 | 64.610 | 25.582 | 27.957 | 1.00 98.40 | 7 |
| | END | | | | | | | | | |

| <u>Atom</u> | | | | | | | | | | |
|-------------|------------------|----------|----------|----------|------------|----------|--|--|--|--|
| <u>Type</u> | <u>Residue #</u> | <u>X</u> | <u>Y</u> | <u>Z</u> | <u>OCC</u> | <u>B</u> | | | | |

20

Table 1: Structural coordinates of AChBP

"Atom type" refers to the element whose coordinate are measured. The first letter in the column defines the element.

"Residue" refers to the amino acid in the AChBP protein sequence, using the standard three letter abbreviations known in the art.

"#" refers to the residue number.

"X, Y, Z" crystallographically define the atomic position, in three-dimensional space, of the element measured.

"OCC" is the occupancy volume.

30 "B" is a thermal factor that measures movement of the atom around its atomic center.

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Claims

1. A water-soluble protein derived from a mollusc being capable of binding a ligand of a ligand-gated receptor.
5
2. The protein of claim 1, wherein the ligand is acetylcholine, gamma-amino-butyric acid (GABA), glycine or serotonin.
3. The protein of claim 2, wherein said protein is a acetylcholine-binding protein (AChBP).
10
4. The protein of any one of claim 1 to 3 which is capable of forming multimers.
5. The protein of any one of claims 1 to 4 which is derived form a Pulmonata species, preferably from a Basommatophora species.
15
6. The protein of any one of claims 1 to 5 comprising an amino acid sequence selected from the group consisting of:
 - (a) an amino acid sequence as depicted in any one of SEQ ID Nos. 2, 4, 6 or 8 or a functional equivalent thereof, or a fragment of at least 5 continuous amino acids thereof;
20
 - (b) an amino acid sequence having at least 30% amino acid identity to the amino acid sequence of any one of SEQ ID Nos. 2, 4, 6 or 8.
- 25 7. A water-soluble ligand binding protein capable of binding a ligand of a ligand-gated receptor and comprising at least 5 continuous amino acids of the aminoacid sequence depicted in any one of SEQ ID Nos. 2, 4, 6 or 8 and/or said protein is detectable by a monoclonal or polyclonal antibody which recognises, preferably with a binding affinity of at least 10^{-7} M, a protein of any one of claims 1 to 6.
30
8. A water-soluble protein being capable of binding a ligand of a ligand-gated receptor comprising
 - (a) at least the amino acids of the water-soluble protein of any one of claims 1 to 6 determining solubility of said protein, in the same or corresponding positions as in said protein; and
35
 - (b) at least 4 amino acids determining binding to said ligand.

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9. The protein of claim 7 or 8 which is capable of forming multimers.
10. The protein of any one of claims 7 to 9 comprising 200-240 amino acids.
- 5 11. The protein of any one of claims 7 to 10, wherein the ligand is acetylcholine, nicotine, lophotoxin, d-tubocurarine, carbamylcholine, galanthamine or epibatidine.
- 10 12. The protein of any one of claims 1 to 11, wherein said ligand-gated receptor is derived from an arthropod (preferably insect), a plant (preferably a higher plant, most preferably a seed plant) or a chordate (preferably a mammalian, most preferably human).
- 15 13. The protein of any one of claims 7 to 12, wherein said ligand-gated receptor is a nicotinic acetylcholine receptor.
- 20 14. The protein of any one of claims 7 to 13, wherein said amino acids determining solubility are in the same positions as in the AChBP having the amino acid sequence as depicted in any one of SEQ ID Nos. 2, 4, 6 or 8; preferably in which said solubility-determining amino acids comprise solvent accessible regions in the crystal structure according to Figure 10.
- 25 15. The protein of any one of claims 7 to 14 comprising an amino acid sequence having at least 40% amino acid identity to the amino acid sequence 20-223 of any one of SEQ ID Nos. 2, 4, 6 or 8, in which the ligand binding amino acids have been replaced with the corresponding amino acids of a ligand-gated receptor.
- 30 16. The protein of any one of claims 7 to 15, in which said solubility-determining amino acids (a) comprise hydrophilic amino acids (Asp, Glu, Arg, Lys) from the sequences 20-44, 73-81, 86-92, 112-120, 135-152, 166-189, 196-20, 209-213, and/or 219-227 of SEQ ID No. 2.
- 35 17. The protein of claim 16, in which said solubility determining amino acids (a) comprise amino acids Asp(36), Asp(68), Glu(115), Arg(137), Asp(143), Asp(148), Glu(150), Arg(167), Arg(189), Glu(215) of SEQ ID No.2, wherein

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Asp may be exchanged for Glu and vice versa and Lys may be exchanged for Arg and vice versa.

- 5 18. The protein of any one of claims 7 to 17 which further comprises the amino acids Cys(142), Thr(149), Ala(153), Thr(154), Cys(155), Arg(156), Ile(157) and/or Lys(158) of SEQ ID No. 2.
- 10 19. The protein of any one of claims 7 to 17 which comprises the amino acids (b) Pro(39), Trp(77), Trp(101), Pro(103), Asp(194), and/or Ser(161) of SEQ ID No. 2.
- 15 20. The protein of any one of claims 7 to 19 in which the amino acid sequences 165-169 and/or 200-203 of SEQ ID No. 2 have been exchanged with the corresponding sequence of the ligand-gated receptor.
- 20 21. The protein of any one of claims 7 to 20 which is capable of binding a ligand of an acetylcholine receptor, in which at least one of the amino acid sequences Trp(101) - Tyr(T08), Trp(162) - His(164) and Tyr(204) - Tyr(211) of SEQ ID No. 2 have been exchanged with the corresponding sequence of the acetylcholine receptor.
- 25 22. A method for the production of a water-soluble ligand-gated receptor or a corresponding ligand-binding domain or for improving the water solubility and accessibility to crystallization of such a receptor or domain, said method comprising altering the amino acid sequence of the extracellular domain of a ligand-gated receptor by way of substituting, adding, deleting or modifying at least one amino acid at a position corresponding to an amino acid determining or contributing to the water-solubility of the protein of any one of claims 1 to 21.
- 30 23. The method of claim 22, wherein the ligand-gated receptor is defined as in any one of claims 1 to 21.
- 35 24. The method of claim 22 or 23, wherein at least one amino acid is altered to the corresponding amino acid of the amino acid sequence depicted in any one of SEQ ID Nos. 2, 4, 6 or 8, or to a an equivalent amino acid, preferably

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in which said solubility-determining amino acids comprise solvent accessible regions in the crystal structure according to Figure 10.

- 5 25. The method of any one of claims 22 to 24, wherein loop Cys123-Cys136 of SEQ ID No. 2 is inserted into the corresponding region of the ligand binding domain of the ligand-gated receptor.
- 10 26. The method of any one of claims 22 to 25 further comprising
 (a) culturing a host cell transfected with and capable of expressing a polynucleotide comprising a nucleotide sequence encoding the altered amino acid sequence; and optionally
 (b) recovering said water-soluble ligand-gated receptor or corresponding ligand-binding domain from the culture.
- 15 27. A water-soluble ligand-gated receptor or ligand-binding domain obtainable by the method of any one of claims 22 to 26.
- 20 28. The protein of any one of claims 1 to 21 or 27 further comprising a spacer sequence allowing coupling with a carrier body.
29. A fusion protein comprising the water-soluble ligand-binding protein of any one of claims 1 to 21, 27 or 28, or a binding fragment thereof and a fragment of a ligand-gated receptor
- 25 30. A dimer or pentamer consisting of at least one monomer comprising a protein of any one of claims 1 to 21 or 27 to 29.
- 30 31. A ligand-gated ion channel comprising a protein of any one of claims 1 to 21 or 27 to 29 or the dimer or pentamer of claim 30.
32. One or more polynucleotides encoding the protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30 or the ligand-gated ion channel of claim 31.
- 35 33. The polynucleotide(s) of claim 32 which comprise(s)

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- (a) a nucleotide sequence having at least 15 continuous nucleotides of the nucleotide sequence depicted in any one of SEQ ID Nos. 1, 3, 5 or 7 or a degenerated sequence thereof; or
- (b) a nucleotide sequence capable of hybridizing to a nucleotide sequence of (a) under stringent hybridisation conditions.
34. The polynucleotide(s) of claim 32 or 33 which is(are) operatively linked to heterologous expression control sequences allowing expression in prokaryotic or eukaryotic cells.
35. One or more vector(s) containing the polynucleotide(s) of any one of claims 32 to 34.
36. A host cell genetically engineered with the polynucleotide(s) of any one claims 32 to 34 or with the vector(s) of claim 35.
37. An antigen comprising an epitope of at least 5 continuous amino acids of the amino acid sequence depicted in any one of SEQ ID Nos. 2, 4, 6 or 8 and/or said epitope is detectable by a monoclonal or polyclonal antibody which recognises, preferably with a binding affinity of at least $10^{-7}M$, a protein of any one of claims 1 to 6.
38. An antibody specifically recognizing the protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30, the ligand-gated ion channel of claim 31 or the antigen of claim 37.
39. An oligonucleotide probe comprising a nucleotide sequence having at least 15 continuous nucleotides of a polynucleotide of any one claims 32 to 34 or encoding the antigen of claim 37.
40. A composition comprising the protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30, the ligand-gated ion channel of claim 31, the polynucleotide(s) of any one claims 32 to 34, the vector(s) of claim 35, the host cell of claim 36, the antigen of claim 37, the antibody of claim 38, or an oligonucleotide probe of claim 39; and optionally suitable means for detection or performing a ligand-receptor binding assay.

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41. A method for identifying an agonist/activator or antagonist/inhibitor of a ligand-gated receptor comprising the steps of:
- 5 (a) contacting the water-soluble ligand-binding protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30, the ligand-gated ion channel of claim 31 or a cell expressing said protein in the presence of components capable of providing a detectable signal in response to ligand binding with a compound to be screened under conditions that permit binding of said compound to the ligand-binding protein; and
- 10 (b) detecting the presence or absence of a signal generated from the binding activity of the ligand-binding protein, wherein the presence/increase and absence/decrease of the signal is indicative for an agonist/activator and antagonist/inhibitor, respectively, of a ligand-gated receptor.
- 15 42. A crystal of a protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30 or the ligand-gated ion channel of claim 31.
- 20 43. A crystal of a protein-ligand complex comprising a protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30 or the ligand-gated ion channel of claim 31; and a ligand.
- 25 44. The crystal of claim 43, wherein the ligand comprises an N-alkylated hydroxyalkyl and/or a quaternary ammonium ion.
- 30 45. The crystal of claim 43, wherein the ligand comprises 4-(2-Hydroxyethyl)-1-piperazineethanesulfonic acid (HEPES), B-bippinatin, lophotoxin, d-tubocurarine, carbamylcholine, galanthamine, epibatidine or alpha-bungarotoxin.
- 35 46. The crystal of any one of claims 42 to 45, wherein the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein or protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms.
47. The crystal of any one claims 42 to 46, wherein the protein has an amino acid sequence of amino acids 20 to 223 of SEQ ID No. 2, or an amino acid

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sequence that differs from amino acid 20 to 223 of SEQ ID No. 2 by only having conservative substitutions.

48. The crystal of claim 47, wherein the ligand is HEPES.
- 5
49. The crystal of claim 46 having (1) a space group of $P2_12_12_1$ and a unit cell of dimensions of $a=120.6\text{\AA}$, $b=137.0\text{\AA}$ and $c=161.5\text{\AA}$; (2) a space group of $P4_22_12$ and a unit cell of dimensions of $a=b=141.6\text{\AA}$ and $c=120.8\text{\AA}$ or (3) a space group of $P2_1$ and a unit cell of dimensions of $a=121.1\text{\AA}$, $b=162.1\text{\AA}$, $c=139.4\text{\AA}$, $\beta=90.1^\circ$.
- 10
50. The crystal of any one of claims 42 to 49, wherein the protein has secondary structural elements that include α -helix and antiparallel β -sheets as shown in Figure 7, 10, 11 and/or 12.
- 15
51. The crystal of any one claims 42 to 50 having a three-dimensional structure as defined by atomic coordinates shown in Table 1.
52. The crystal of any one of claims 42 to 51 having a binding cavity as shown in Figure 6, 8, 9 and/or 13.
- 20
53. A method of using the crystal of any one of claims 42 to 52 in a drug screening assay comprising:
- 25
- (a) selecting a potential ligand by performing structure assisted drug design with the three-dimensional structure determined for the crystal, wherein said selecting is performed in conjunction with computer modeling; optionally
- (b) contacting the potential ligand with the ligand binding domain of the ligand-gated receptor in an in vitro or in vivo assay; and
- 30
- (c) detecting the binding of the potential ligand for the ligand binding domain.
54. The method of claim 53, wherein the ligand-gated receptor is a nicotinic acetylcholine receptor.
- 35
55. The method of claim 53 or 54 further comprising:

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- 5 (d) forming a supplemental crystal of a protein-ligand complex by co-crystallization or soaking the crystal of the water-soluble ligand-binding protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30 or the ligand-gated ion channel of claim 31, with a potential drug, wherein the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms, more preferably greater than 3;
- 10 (e) determining the three-dimensional structure of the supplemental crystal;
- (f) selecting a candidate drug by performing a structure assisted drug design with the three-dimensional structure determined for the supplemental crystal, wherein said selecting is performed in conjunction with computer modeling; optionally
- 15 (g) contacting the candidate drug with a cell that expresses the ligand-gated receptor; and
- (h) detecting a cell response; wherein a candidate drug is identified as a drug when the cell response is altered compared to a cell that has not been contacted with the candidate compound.
- 20
56. The method of any one of claims 53 to 55 further comprising an initial step that precedes step (a) wherein said initial step consists of determining the three-dimensional structure of a crystal comprising a protein-ligand complex formed between the water-soluble ligand-binding protein of any one of claims
- 25 1 to 21 or 27 to 29, the dimer or pentamer of claim 30 or the ligand-gated ion channel of claim 31, and the ligand of the ligand-gated receptor, wherein the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms.
- 30
57. A method of growing a crystal of a protein-ligand complex comprising:
- (a) contacting the water-soluble ligand-binding protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30 or the
- 35 ligand-gated ion channel of claim 31 with a ligand of a ligand-gated receptor, wherein the water-soluble ligand-binding protein forms a protein-ligand complex with the ligand; and

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- (b) growing the crystal of the protein-ligand complex; wherein the crystal effectively diffracts X-rays for the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 5.0, preferably greater than 4.0 Angstroms.

5

58. A drug screening assay comprising soaking the crystal of any one of claims 42 to 52 in a solution of compounds to be screened and detecting the binding of the compound to the ligand-binding protein.

10

59. The method of claim 57 or 58, wherein said ligand comprises an alkylated nitrogen and/or quaternary ammonium ion.

60. A method of increasing or decreasing the affinity of a drug to a ligand-gated receptor, comprising

15

- (a) performing structure assisted drug design with the three-dimensional structure determined for the crystal of any one of claims 42 to 52, wherein said drug design is performed in conjunction with computer modeling; and

20

- (b) modifying said drug to alter or eliminate a portion thereof suspected of interacting with a binding site of the binding cavity or with a non-specific binding site of the protein in the crystal.

61. The method of claim 60, wherein step (a) further comprises the steps of a method of any one of claims 53 to 59.

25

62. The method of claim 60 or 61, further comprising after step (b), the additional step of:

- (c) repeating the method used to perform structure assisted drug design according to step (a) using the modified drug according to step (b).

30

63. A method of drug design comprising the step of using the structural coordinates of a water-soluble ligand-binding protein crystal comprising the coordinates of Table 1, to computationally evaluate a chemical entity for associating with the ligand-binding site or a non-specific binding site of a ligand-binding protein.

35

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64. The method of any one of claims 53 to 63, wherein the identified drug prevents or promotes correct assembly of a ligand-gated ion channel.
- 5 65. The method of any one of claims 53 to 63, wherein the identified drug binds to a non-specific binding site of a ligand-gated ion channel.
66. The method of any one of claims 53 to 65 further comprising synthesizing the drug in a therapeutically effective amount.
- 10 67. A drug produced by the method of claim 66 or a pro-drug thereof.
68. The drug of claim 67 which interacts with a ligand-gated receptor comprising a pentamer of claim 30 with monomers A to E, wherein the drug binds to one or more primary contact regions of a monomer (residues from A contacting B) defined by amino acid residues 15 to 21, 44 to 47, 85 to 87, 91 to 94, 122 to 124, 143 to 146, 149, 185 to 187 of the mature protein of SEQ ID No. 2 and/or to one or more of the complementary contact regions of the other monomer (from B contacting A, (identical to residues on A contacting E) defined by amino acid residues 3 to 4, 7 to 8, 11, 37 to 39, 53, 75 to 77, 96 to 104, 114 to 118 and 163-170 of the mature protein of SEQ ID No. 2; or to the contact regions as identified in Figure 14; or to the corresponding contact regions of the monomers of a ligand-gated ion channel.
- 15 20
69. The drug of claim 68, wherein the ligand-gated ion channel is the nicotinic acetylcholine receptor and the order of the monomers is $\alpha\gamma\alpha\beta\delta$.
- 25
70. A computer readable medium comprising a nucleotide sequence of the polynucleotide(s) of any one of claims 32 to 34, an amino acid sequence of a protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30 or the ligand-gated ion channel of claim 31, or the structural coordinates of a crystal of any one of claims 40 to 50.
- 30
71. A device comprising the computer readable medium of claim 70.
- 35 72. Use of the computer readable medium of claim 70 or the device of claim 71 for modeling an antagonist/inhibitor or agonist/activator of a ligand-gated receptor.

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73. Use of the crystal of any one of claims 42 to 52 or its structural coordinates as a template for modeling the 3D structure of a ligand-gated ion channel.
- 5 74. Use of the polynucleotide(s) of any one of claims 32 to 34, the protein of any one of claims 1 to 21 or 27 to 29, the dimer or pentamer of claim 30, the ligand-gated ion channel of claim 31, the vector(s) of claim 35, the host cell of claim 36, the antigen of claim 37, the antibody of claim 38, an oligonucleotide probe of claim 39, the crystal of any one of claims 42 to 52 or a method of any
10 one of claims 53 to 66 for screening or profiling putative ligands of ligand-gated receptors.
75. Use of an antagonist/inhibitor or agonist/activator identified according to a method of any one of claims 53 to 66 for the preparation of a pharmaceutical
15 composition for the treatment of a ligand-gated ion channel mediated or related disorder.
76. The use of claim 75, wherein the antagonist/inhibitor is or is derived from the protein of any one of claims 1 to 21 or 27 to 29, an antigen of claim 37, an
20 antibody of claim 38 or from a toxin of the ligand-gated ion channel.
77. The use of claim 75, wherein the agonist/activator is or is derived from a the protein of any one of claims 1 to 21 or 27 to 29, an antigen of claim 37, an antibody of claim 38 or from epibatidine, acetylcholine, choline, nicotine,
25 carbachol, serotonin or GABA.
78. The use of any one claims 75 to 77, wherein the ligand-gated ion channel is the nicotinic acetylcholine receptor and said mediated or related disorder is Tourette's syndrome, Alzheimer's disease, addiction to nicotine or
30 schizophrenia.
79. Use of ligand of a ligand-gated receptor for identifying and isolating a water-soluble ligand-binding protein from a mollusc.
- 35 80. The use of claim 79, wherein said ligand is α -bungarotoxin.

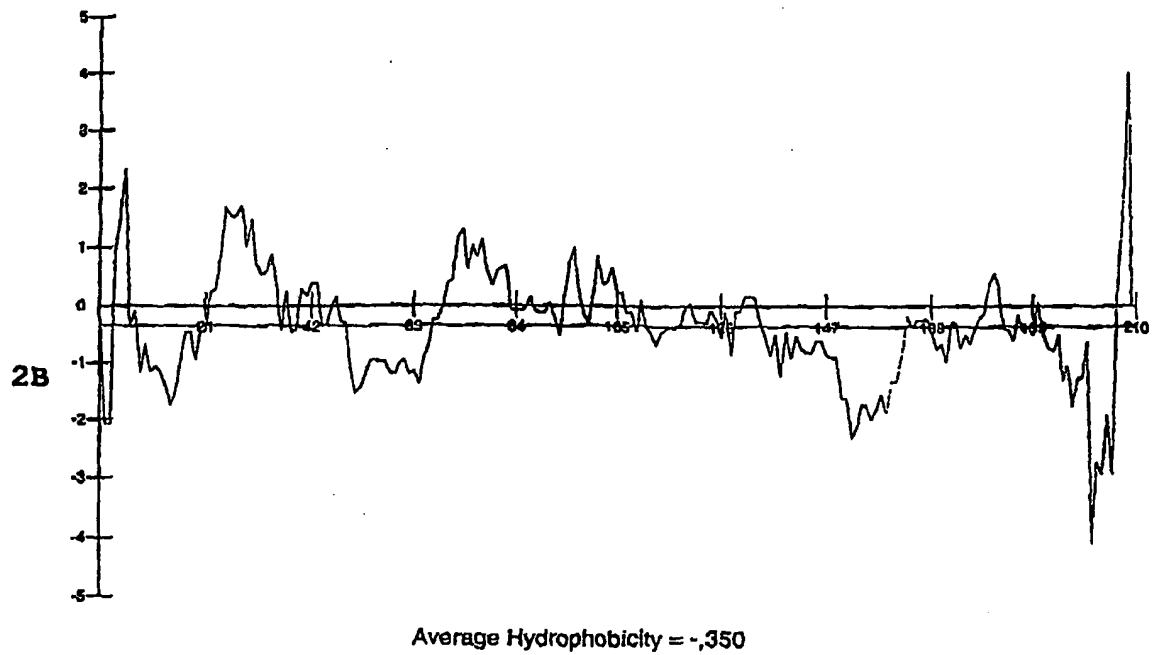
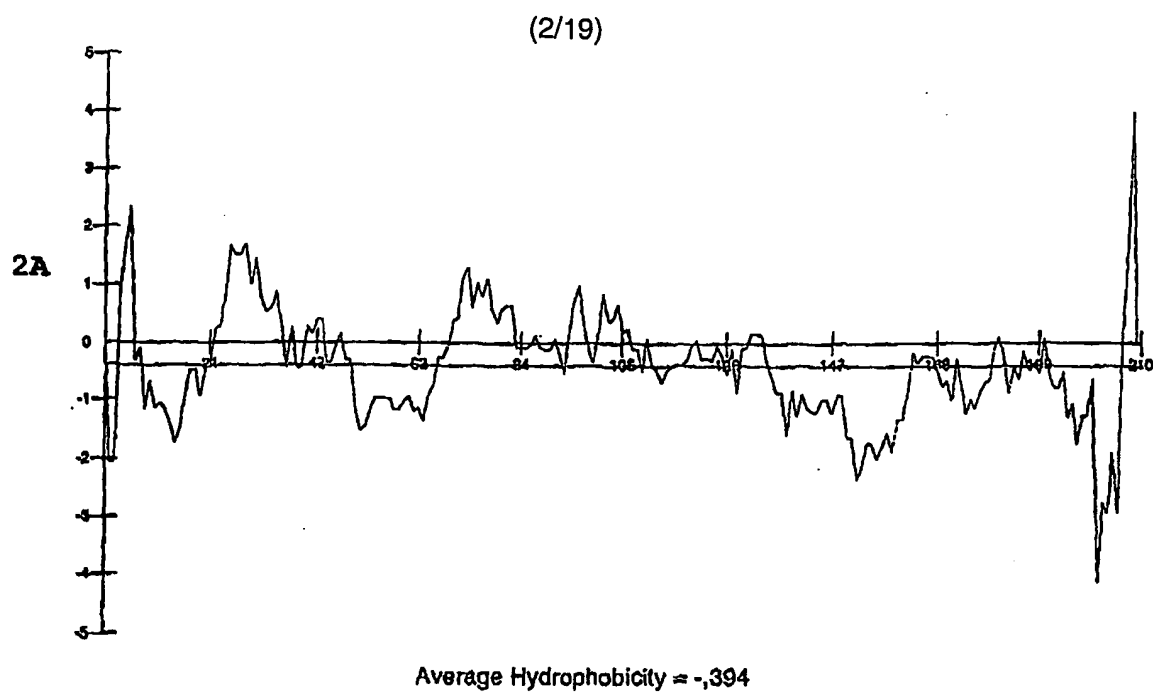

```
L-AChBP_T1. --MRRNIFCLACLWIVQACLSLDRADILYNIROTSPDVPTQRDRPVAVSVSLKFINIL
L-AChBP_T2. --MRRNIFCLACLWIVQGCLSLDRADILYNIROTSPDVPTQRDRPVAVSVSLKFINIL
B-AChBP_T1. MAELRRIILLCTIAFHVSHGQIRWTLLNQITGES--DVIPLSNNTPLNVSLNFKL MNIV
B-AChBP_T2. MAELRGIILLCTIAFHVSHGQIRWTLLNQITGES--DVIPLSNNTPLNVSLNFKL MNIL
          * *: * * . : . . * ; * * * * * .. : * : * : : * : * :

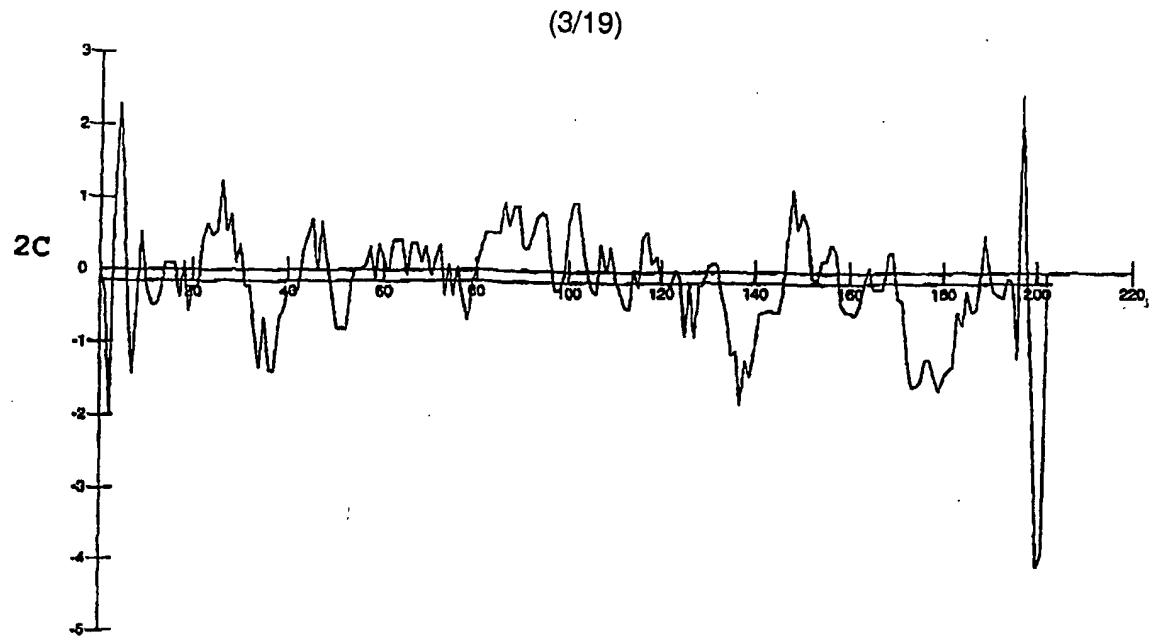
L-AChBP_T1. EVNEITNEVDVVFWQQTTSWRDLA-WNSSHSPDQVSVPISSSLWVPDLAAYN AISKP EVL
L-AChBP_T2. EVNEITNEVDVVFWQQTTSWRDLA-WNSSHSPDQVSVPISSSLWVPDLAAYN AISKP EVL
B-AChBP_T1. EADTEKDQVEVVLWTOASWKVPYSSLLSSSSLDQVSLPVMKWTPDLSFYNAIAAPELL
B-AChBP_T2. EADTEKDQVEVVLWTOASWKVPYSSLLSSSSLDQVSLPASKMWTPDLSFYNAIAAPELL
          *.: . :*: *:* * * :*. : * * * * * :* :*. * :*. * :*. * :*. * :*

L-AChBP_T1. TPQLARVSDGEVLYMPSIRQRFSCDVGVDTESGATCRIKIGSWTHHSREISVDPTTE-
L-AChBP_T2. TPQLARVSDGEVLYMPSIRQRFSCDVGVDTESGATCRIKIGSWTHHSGEISVDPTTE-
B-AChBP_T1. SADRVVSVSKDGSVIYVPSQVRVFTCDLINVDTEPGATCRIKVGSWTHDNKQFALITGEEG
B-AChBP_T2. STDRVVSVSKDGSVIYVPSQVRVFTCDLINVDTEPGATCRIKVGSWTFDNKQLALITGEEG
          :.: . * . **.*: * * * **:*. :****.*****:* ****... ::: . *

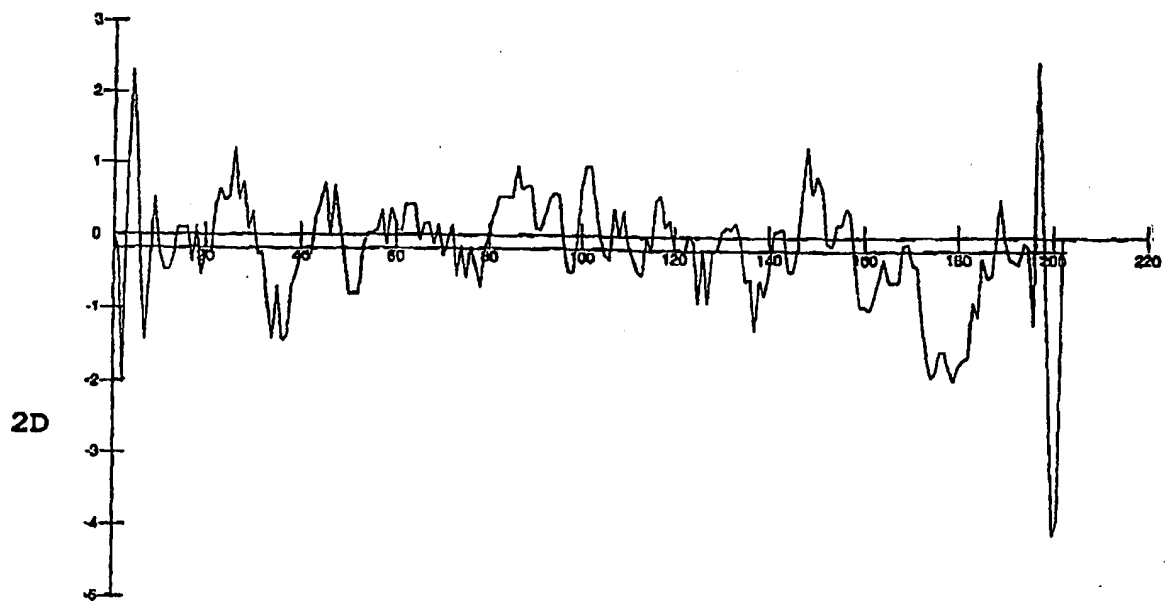
L-AChBP_T1. NSDDSEYFSQYSRFEILDVTQKN SVTYSCCPEAYEDVEVSLNFRKKGRSEIL
L-AChBP_T2. NSDDSEYFSQYSRFEILDVTQKN SVIYSCCPEAYEDVEVSLNFRKKGRSEIL
B-AChBP_T1. VVNIAEYFDS-PKFDDL SATQS LNRKKYSCCENMYDDIEITFAFRKK-----
B-AChBP_T2. VVNIAEYFDS-PKYDLLS ATQS LNRKKYRCENMYEDIEITFAFRKK-----
          : :***. : * : * : * : * : * : * : *
```

Figure 1

**Figure 2**



Average Hydrophobicity = -,159



Average Hydrophobicity = -,189

Figure 2 (continued)

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L-AChBP_T1 -----LDRADILYNIRQTSRPDVIPT
L-AChBP_T2 -----LDRADILYNIRQTSRPDVIPT
B-AChBP_T1 -----QIRWTLNQTIGES--DVIPL
B-AChBP_T2 -----QIRWTLNQTIGES--DVIPL
h_nAChR_A7 -----MRCSPGGVWLALAAASLLHV-----SIQGEFQRKLYKELVKYNPLERP
h_5HT3 -----MLLWVQQALLALLPTLLAQGEARRSRNTRPALLRLSDYLLTNYRKGVPRV
h_GlyR_a1 -MYSFNTLRRLYLSGAIVFFSLAASKEAEAARSATKPMSPSDFLDKLMGRTSGYDARIRPN
h_GABAA_b1 MRKSPGLSDCLWAWILLSTLTGRSYGQPSLQDELKDNTTVFTRILDRLLDGYDNRLRPG
*

L-AChBP_T1 QRDR-PVAVSVSLKFINILEVNEITNEVDVVFQQTTWSDRTLA--WNSSHSPDQVSVPI
L-AChBP_T2 QRDR-PVAVSVSLKFINILEVNEITNEVDVVFQQTTWSDRTLA--WNSSHSPDQVSVPI
B-AChBP_T1 SNNT-PLNVSLNFKLMNIVEADTEKDQVEVVLWTQASWKVPYYSS-LLSSSLDQVSLPV
B-AChBP_T2 SNNT-PLNVSLNFKLMNILEADTEKDQVEVVLWTQASWKVPYYSS-LLSSSLDQVSLPA
h_nAChR_A7 ANDSQPLTVYFSLSLQIMDVDEKNQVLTNNIWLQMSWTDHYLQWNVSEYPGVKTVRFPD
h_5HT3 RDWRKPTTVSIDVIVYAILNVDEKNQVLTYYIWRQYWTDEFLQWNPEDFNITKLSIPT
h_GlyR_a1 FKGP-PVNVSCNIFINSFGSIAETMDYRVNIFLRQQWNPRLAYNEYPDSDLDPDPSML
h_GABAA_b1 LGER-VTEVKTDIFVTSFGPVSDDHMEYTDVFFRQSWKDERLKF-KGPMTVLRLNNLMA
* . . . : . . . *

L-AChBP_T1 SSLWVPDLAAYNAISK-PEVLTPQ--LARVVS DGEVLYMPSIRQRFSCDVSG-VDTESGA
L-AChBP_T2 SSLWVPDLAAYNAISK-PEVLTPQ--LARVVS DGEVLYMPSIRQRFSCDVSG-VDTESGA
B-AChBP_T1 SKMWT PDL SFYNAIAA-PELLSAD--RVVVS KDGSVIYVPSQRVRFTCDLIN-VDTEPGA
B-AChBP_T2 SKMWT PDL SFYNAIAA-PELLSTD--RVVVS KDGSVIYVPSQRVRFTCDLIN-VDTEPGA
h_nAChR_A7 GQIWKP DILLYNSADERFDATFHT--NVLVNSSGHCQYLPPIGFKSSCYIDVRWFPPDVQ
h_5HT3 DSIWVP DILINEFVDV-GKSPNIP--YVYIRHQGEVQNYKPLQVVTACSLDIYNFPFDVQ
h_GlyR_a1 DSIWKP DLF FANEKGAFHEITTDNKLRLISRNGNVLYSIRITLT LACPM D LKNFPM D VQ
h_GABAA_b1 SKIRTPDTFFHNGKKSVAHNMTMPNKLRLITEDGTLTYMRLTVRAECPMHLEDFPMDAH
... ** : . . . *

L-AChBP_T1 TCRIKIGSWTHHSREISVDPT---TE-NSDDSEYFSQYSRFEILDVTQKKNSVTYSCCPE
L-AChBP_T2 TCRIKIGSWTHHSREISVDPT---TE-NSDDSEYFSQYSRFEILDVTQKKNSVTYSCCPE
B-AChBP_T1 TCRIKIGSWTHDNKQFALITG---EEGVVNIAEYFDS-PKFDLLSATQSLNRKKYSCCEN
B-AChBP_T2 TCRIKIGSWTFDNKQFALITG---EEGVVNIAEYFDS-PKYDLLSATQSLNRKKYSCCEN
h_nAChR_A7 HCKLKFGSWSYGGWSLDLQMQ---EA---DISGYIPN-GEWDLVGIPGKRSEFYECCKE
h_5HT3 NCSLTFTSWLHTIQDINISLWRLPEKVKSDRSVEMNQ-GEWELLGVLPYFREFSMESS-N
h_GlyR_a1 TCIMQLESFGYTMNDLIFEWQ---EQGAVQVADGLTL-PQFILKEEKDLRYCTKHNT-G
h_GABAA_b1 ACPLKFGSYAYTRAEVVYEWTR-EPARSVVVAEDGSRLNQYDLLG--QTVDSGIVQSSTG
* : . * : . . . : . . .

L-AChBP_T1 AYEDVEVSLNFRKKGRSEIL
L-AChBP_T2 AYEDVEVSLNFRKKGRSEIL
B-AChBP_T1 MYDDIEITFAFRKK-----
B-AChBP_T2 MYEDIEITFAFRKK-----
h_nAChR_A7 PYPDVTFTVTMRRRTLYYGL
h_5HT3 YYAEMKFYVVIRRRPLFYVV
h_GlyR_a1 KFTCIEARFHLERQMGYYLI
h_GABAA_b1 EYVVMTHFHLKRRKIGYFVI
: : . . . :

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Figure 3

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nAchR_h-A2      MGPSCPVFLSFTKLSLWLLLLT PAGGEEAKRPPPRAPGDP---LSSPSETALPQGGSHTE
nAchR_h-A4      -----MELGGPGAPRLLP-----P---LLLLLTGTLRASSHVE
nAchR_h-A5      -----MAARGSGPRALRLLLLVQLVAGRCGLAGAAGGAQRGLSEPS
nAchR_h-A3      -----MALAALAAPGAVAPRLLL-----LLLSLLP--VAR---ASE
nAchR_h-A6      -----MLTSKGQGFHLGGCL-----WLCVFTP--FFKGCVGCA
nAchR_h-A1      -----MEPWPLLL-----LFSLCSAGLVLG---SE
nAchR_h-A7      -----MRCSPGGVWLALAASL-----LHVS LQG-EFQR-----
nAchR_h-A9      -----CISFCWIYFAASRLR-----AAETADG-KYAQ-----
B-AchBP_T1      -----MAELRRIILLCT-----IAFHVSHG-QIR-----
B-AchBP_T2      -----MAELRGIILLCT-----IAFHVSHG-QIR-----
L-AchBP_T1      -----MRRNIFCLACL-----WIVQACLS-LDR-----
L-AchBP_T2      -----MRRNIFCLACL-----WIVQGCLS-LDR-----

nAchR_h-A2      T----EDRLFHKLFRGYNRWARVPVNTSDVIVRFGLSIAQLIDVDEKNQMMTTNVWLKQ
nAchR_h-A4      TRAHAEERLLKKLFSGYNKSRPVANISDVVLRVFGLSIAQLIDVDEKNQMMTTNVWLKQ
nAchR_h-A5      SIAKHEDSLLKDLFQDYERWVRPVEHLNDKIKIKFGLAISQLVDVDEKNQMMTTNVWLKQ
nAchR_h-A3      A----EHLRFERLFEDYNEIIRPVANVSDPVIHFEVMSQLVKVDEVNQIMETNLWLKQ
nAchR_h-A6      T----EERLFHKLFSHYNQFIRPVENVSDPVTVHFEVAITQLANVDEVNQIMETNLWLRR
nAchR_h-A1      H----ETRLVAKLFKDYSSVVRPVEDHRQVVEVTVGLQLIQLINVDEVNQIVTTNVRLKQ
nAchR_h-A7      -----KLYKELVKKNYNPLERPVANSDSPLTVYFSLSLQIMDVDEKNQVLTNNIWLQM
nAchR_h-A9      -----KLFNDLFEDYSNALRPVEDTDKVLNVTLQITLSQIKDMERNQILTAYLWIRQ
B-AchBP_T1      -----WTLLNQITGES--DVIPLSN-NTPLNVSLNFKLMNIVEADTEKDQVEVVLWTQA
B-AchBP_T2      -----WTLLNQITGES--DVIPLSN-NTPLNVSLNFKLMNILEADTEKDQVEVVLWTQA
L-AchBP_T1      -----ADILYNIRQTSRPDVIPTQR-DRPVAVSLSLKFINILEVNEITNEVDVVFQQQT
L-AchBP_T2      -----ADILYNIRQTSRPDVIPTQR-DRPVAVSLSLKFINILEVNEITNEVDVVFQQQT
                :      :      *      :      :      :      :      :      :

nAchR_h-A2      EWS DYKLRWNPTDFGNITSLRVPSEMIWIPDIVLYNNADGEFAVTHMTKAHLSTGTVHW
nAchR_h-A4      EWHDYKLRWDPADYENVTSIRIPSELIWRPDI VLYNNADGDFAVTHLTKAHLFHDGRVQW
nAchR_h-A5      EWI DVKLRWNPDDYGGIKVIRVPSDSVWTPDIVLFDNADGRFEGTS-TKTVIRYNGTWTW
nAchR_h-A3      IWNDYKLRWNP SDYGGAEFMRVPAQKIWKPDIVLYNNAVGDFQVDDKTKALLKYTG EVTW
nAchR_h-A6      IWNDYKLRWDPMEYDGIETLRVPADKIWKPDIVLYNNAVGDFQVEGKTKALLKYNGMITW
nAchR_h-A1      QWVDY NLKWNPDYGGVKKIHIPESEKIWRPDLVLYNNADGDFAI VKTKVLLQYTGHTW
nAchR_h-A7      SWT DHYLQWNVSEYPGVKTVRFDPDGIWKPDILLYNSADERFDATFHTNVLVNSSGHCQY
nAchR_h-A9      IWHDAYLTWRDQYDGLDSIRIPSDLVWRPDI VLYNKADDESSEPVNTNVVLRDGLITW
B-AchBP_T1      SWKV PYYSS--LLSSSSLDQVSLPVS KMWTPDLSFYN-AIAAPELLSADR VVSKDGSVIY
B-AchBP_T2      SWKV PYYSS--LLSSSSLDQVSLPASKMWT PDLSFYN-AIAAPELLSTDR VVSKDGSVIY
L-AchBP_T1      TWS DRTL A--WNSSHSPDQVSVPISSLWVPDLAAYN-AISKPEVLT PQLARVVS DGEVLY
L-AchBP_T2      TWS DRTL A--WNSSHSPDQVSVPISSLWVPDLAAYN-AISKPEVLT PQLARVVS DGEVLY
                *      .      :      *      :      *      :      :      :

nAchR_h-A2      VPPAIYKSSCSIDVTFFPFDDQNCMKFGSWTYDKAKIDLEQMEQ-TVDLKDYWES-GEW
nAchR_h-A4      TPPAIYKSSCSIDVTFFPFDDQNCMTMKFGSWTYDKAKIDLVMHS-RVDQLDFWES-GEW
nAchR_h-A5      TPPANYKSSCTIDVTFFPFDDLQNCMKFGSWTYDGSQVDIILEDQ-DVDKRDFFDN-GEW
nAchR_h-A3      IPPAIFKSSCKIDVTYFFFDYQNCMTMKFGSWSYDKAKIDLVLIGS-SMNLKDYWES-GEW
nAchR_h-A6      TPPAIFKSSCPMDITFFPFDHQNC SLKFGSWTYDKAEIDLLIGS-KVDMNDFWEN-SEW
nAchR_h-A1      TPPAIFKSYCEIIVTHFPFDEQNCMKLGTWYTDGSVVAINPESD-QPDL SNFMES-GEW
nAchR_h-A7      LPPGIFKSSCYIDVRWFPPFDVQHCKL KFGSWSYGGWSLDLQM--Q-EADISGYIPN-GEW
nAchR_h-A9      DAPAITKSSCVVDVTYFFFDNQNCNLTFGSWTYNGNQVDIFNALD-SGDLSDFIED-VEW
B-AchBP_T1      VPSQRVRFTCDLINVDTEPG-ATCRIKVGSWTHDNKQFALITGEEGVVNI AEYFDS-PKY
B-AchBP_T2      VPSQRVRFTCDLINVDTEPG-ATCRIKVGSWTHDNKQFALITGEEGVVNI AEYFDS-PKY
L-AchBP_T1      MPSIRQRFSCDVSGVDTESG-ATCRIKIGSWTHHSREISVDP TTE-NSDDSEYFSQYSRF
L-AchBP_T2      MPSIRQRFSCDVSGVDTESG-ATCRIKIGSWTHHSREISVDP TTE-NSDDSEYFSQYSRF
                ..      :      *      :      .      *      :      :      :      :

```

Figure 4

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| | |
|------------|--|
| nAChR_h-A2 | AIVNATGTYNSSKKYDCCAE-IYPDVTYAFVIRRLPLFYTTINLIIPCLLISCLTVLVFYLP |
| nAChR_h-A4 | VIVDAVGTYNTRKYECACAE-IYPDITYAFVIRRLPLFYTTINLIIPCLLISCLTVLVFYLP |
| nAChR_h-A5 | EIVSATGSKGNRTDSCC---WYPYVTYSFVIKRLPLFYTLFLIIPCIGLSFLTVLVFYLP |
| nAChR_h-A3 | AI IKAPGYKHDIKYNCCCE-IYPDITYSLYIRRLPLFYTTINLIIPCLLISFLTVLVFYLP |
| nAChR_h-A6 | EI IDASGYKHDIKYNCCCE-IYTDITYSFYIRRLPMFYTTINLIIPCLFISFLTVLVFYLP |
| nAChR_h-A1 | VIKESRGWKHSVTYSCCPDTPYLDITYHFVMQRLPLYFIVNVIIPCLLFSFLTGLVFYLP |
| nAChR_h-A7 | DLVGIPGKRSERFYECCKE-PYPDVTFTVTMRRRTLYYGLNLLIPCVLISALALLVFLLP |
| nAChR_h-A9 | EVHGMPAVKNVISYGCCSE-PYPDVTFTLLKRRSSFYIVNLLIPCVLISFLAPLSFYLP |
| B-AChBP_T1 | DLLSATQSLNRKKYSCCEN-MYDIEITFAFRKK----- |
| B-AChBP_T2 | DLLSATQSLNRKKYSCCEN-MYDIEITFAFRKK----- |
| L-AChBP_T1 | EILDVTQKKNSVTYSCCPE-AYEDVEVSLNFRKKGRSEIL----- |
| L-AChBP_T2 | EILDVTQKKNSVIYSCCPE-AYEDVEVSLNFRKKGRSEIL----- |
| | : ** * : . ::: |
| | |
| nAChR_h-A2 | SDCGEKITLCISVLLSLTVFLLLITEIIPSTSLVIPLIGEYLLFTMIFVTLISIVITVFVL |
| nAChR_h-A4 | SECGEKITLCISVLLSLTVFLLLITEIIPSTSLVIPLIGEYLLFTMIFVTLISIVITVFVL |
| nAChR_h-A5 | SNEGEKICLCTSVLVSLTVFLLVIEEIPSSSKVIPLIGEYLVFTMIFVTLISIMTVFAI |
| nAChR_h-A3 | SDCGEKVTLCSVLLSLTVFLLVITETIPSTSLVIPLIGEYLLFTMIFVTLISIVITVFVL |
| nAChR_h-A6 | SDCGEKVTLCSVLLSLTVFLLVITETIPSTSLVPLVGEYLLFTMIFVTLISIVTVFVL |
| nAChR_h-A1 | TDSGEKMTLSISVLLSLTVFLLVIVELIPSTSSAVPLIGKYLFTMVFIASIIITVIVI |
| nAChR_h-A7 | ADSGEKISLGITVLLSLTVFLLVLAIEIMPATSDSVPLIAQYFASTMIIVGLSVVTVIVL |
| nAChR_h-A9 | AASGEKVSGLVTILLAMTVFQLMVAEIMP-ASENVPLIGKYYIATMALITASTALTIMVM |
| B-AChBP_T1 | ----- |
| B-AChBP_T2 | ----- |
| L-AChBP_T1 | ----- |
| L-AChBP_T2 | ----- |
| | |
| nAChR_h-A2 | NVHHRSPSTH-TMPHWVRGALLGCVPRWLLMNRP----- |
| nAChR_h-A4 | NVHHRSPRTH-TMPTWVRRVFLDIVPRLLLMKRPSVVKDNCRRLESMSHKMASAPRFWPE |
| nAChR_h-A5 | NIHHRSSSTHNAMAPLVKIFLHTLPKLLCMRSH----- |
| nAChR_h-A3 | NVHYRTPTTH-TMPSWVKTVFLNLLPRVMFMTRP----- |
| nAChR_h-A6 | NIHYRTPTTH-TMPRWVKTVFLKLLPQVLLMRWP----- |
| nAChR_h-A1 | NTHHRSPSTH-VMPNWRVKVFIDTIPNIMFFSTMK----- |
| nAChR_h-A7 | QYHHHDPDGG-KMPKWTRVILLNWCAWFLRMKRP----- |
| nAChR_h-A9 | NIHFCGAEAR-PVPHWARVVILKYMSRVLFVYDVG----- |
| B-AChBP_T1 | ----- |
| B-AChBP_T2 | ----- |
| L-AChBP_T1 | ----- |
| L-AChBP_T2 | ----- |
| | |
| nAChR_h-A2 | -----PPVELCHPLRLKLSPSYHWLESN-----VDAEEREVVVEEE |
| nAChR_h-A4 | PEGEPPATSGTQSLHPPSPSFCVPLDVPAEPGSPCKSPSDQLPPQPLEAEKASPHPSPG |
| nAChR_h-A5 | -----VDR----- |
| nAChR_h-A3 | -----TSNEGNAQKPRPLYGAELSNNLNCFS-----RAESKGCKEGYPCQ |
| nAChR_h-A6 | -----LDKTRGTGSDAVPRGLARR-----PAKGKLASHGEPRH |
| nAChR_h-A1 | -----RPSREK-----QDKK----- |
| nAChR_h-A7 | -----EDKVRPACQHKQRRCSLAS-----VEMSAVAPPPASN |
| nAChR_h-A9 | -----ESCLSPHHSRER-D-----HLTKVYSKLPESN |
| B-AChBP_T1 | ----- |
| B-AChBP_T2 | ----- |
| L-AChBP_T1 | ----- |
| L-AChBP_T2 | ----- |

Figure 4 (continued)

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| | |
|------------|--|
| nAChR_h-A2 | DRWACAGHVAP-----SVGTLCSHGHLHSG-----ASGPKA |
| nAChR_h-A4 | PCRPPHGTQAPGLAKARSLSVQHMSSPGEAVEGGVRCRSRSIQYCVPRDDAAPEADGQAA |
| nAChR_h-A5 | -----YFTQKEETESG-----SGPKS |
| nAChR_h-A3 | DGMCGYCHHRR--IK--ISNFSANLTRSSSS-----ESVDA |
| nAChR_h-A6 | LKECFHCHK-----SNELATSKRRLSH-----QPLQW |
| nAChR_h-A1 | -----IFTEDIDISDISG-----KPGPPP |
| nAChR_h-A7 | GNLLYIGFRGLDG-----VHCVPTPDSGVVCG-----RMACSPTHD |
| nAChR_h-A9 | LKAARNKDLSR-----KKDMNKRLKNDLG-----CQKGNP |
| B-AChBP_T1 | ----- |
| B-AChBP_T2 | ----- |
| L-AChBP_T1 | ----- |
| L-AChBP_T2 | ----- |

| | |
|------------|--|
| nAChR_h-A2 | EALLQE-----GELLLSPHMOKA |
| nAChR_h-A4 | GALASRNTHSAELPPPQSPCKCTCKKEPSSVSPSATVKTRSTKAPPPHPLPALTRA |
| nAChR_h-A5 | -----SR-----NTLEAA |
| nAChR_h-A3 | VLSLSA-----LSPEIKEA |
| nAChR_h-A6 | VVENSE-----HSPEVEDV |
| nAChR_h-A1 | MGFHSP-----LIKHPEVKSA |
| nAChR_h-A7 | EHLLHGG-----QPPEGDPDLAKI |
| nAChR_h-A9 | QEAESY-----CAQYKVL |
| B-AChBP_T1 | ----- |
| B-AChBP_T2 | ----- |
| L-AChBP_T1 | ----- |
| L-AChBP_T2 | ----- |

| | |
|------------|---|
| nAChR_h-A2 | LEGVHYIADHLRSEDADSSVKEDWKYVAMVIDRIFLWLFIIVCFLGTIGLFLP---PFLA |
| nAChR_h-A4 | VEGVQYIADHLKAEDTDFSVKEDWKYVAMVIDRIFLWMFIIVCLLGTVGLFLP---PWLA |
| nAChR_h-A5 | LDSIRYITRHIMKENDVREVVEDWKFIQVLDRLMFLWTFLEVSIVGSLGLFVPVIYKWAN |
| nAChR_h-A3 | IQSVKYIAENMKAQNEAKEIQDDWKYVAMVIDRIFLWVFTLVCILGTAGLFLQ---PLMA |
| nAChR_h-A6 | INSVQFIAENMKSHNETKEVEDDWKYVAMVVDRLVFLWVFIIVCVFGTAGLFLQ---PLLG |
| nAChR_h-A1 | IEGIKYIAETMKSDQESNNAAEWKYVAMVMDHILLGVFMLVCIIGTLAVFAG---RLIE |
| nAChR_h-A7 | LEEVRVIANRFRQCDESEAVCSEWKFAACVVDRLCLMAFSVFTIICTIGILMSAP-NFVE |
| nAChR_h-A9 | TRNIEYIAKCLKDHKATNSKGSEWKVAKVIDRFFMWIFFIMVFVMTILIIA----- |
| B-AChBP_T1 | ----- |
| B-AChBP_T2 | ----- |
| L-AChBP_T1 | ----- |
| L-AChBP_T2 | ----- |

| | |
|------------|--------------|
| nAChR_h-A2 | GMI----- |
| nAChR_h-A4 | GMI----- |
| nAChR_h-A5 | ILIPVHIGNANK |
| nAChR_h-A3 | REDA----- |
| nAChR_h-A6 | NTGKS----- |
| nAChR_h-A1 | LNQQG----- |
| nAChR_h-A7 | AVSKDFA----- |
| nAChR_h-A9 | ----- |
| B-AChBP_T1 | ----- |
| B-AChBP_T2 | ----- |
| L-AChBP_T1 | ----- |
| L-AChBP_T2 | ----- |

Figure 4 (continued)

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```

B-AChBP_T1. -MAELRRIILLCTIAFHVSHG-QIRWTLNQTIGES--DVIPLSNNT-PLNVSLNFKLM
B-AChBP_T2. -MAELRGIILLCTIAFHVSHG-QIRWTLNQTIGES--DVIPLSNNT-PLNVSLNFKLM
L-AChBP_T1. ---MRRNIFCLACLWIVQACLS-LDRADILYNIRQTSRPDVIPTQRDR-PVAVSVSLKFI
L-AChBP_T2. ---MRRNIFCLACLWIVQGCLS-LDRADILYNIRQTSRPDVIPTQRDR-PVAVSVSLKFI
A1_human --MEPWPLLLLFLCSAGLVLGSEHETRLVAKLFKDYSSVVRPVEDHRQVVEVTVGLQLI
A7_human MRCSPGGVWLGLAASLLHVSLOGEFQRKLYKELVKYNFLERPVANDSQPLTVYFSLSL
      : . . . : : * . : * .....

B-AChBP_T1. NIVEADTEKDQVEVVLWTQASWKVPYYSS-LLSSSSLDQVSLPVSKMWTPLDSFYNAIA
B-AChBP_T2. NILEADTEKDQVEVVLWTQASWKVPYYSS-LLSSSSLDQVSLPASKMWTPLDSFYNAIA
L-AChBP_T1. NILEVNEITNEVDVVFVWQTTWSDRTLA--WNSSHSPDQVSVPISSLWVPDLAAYNAIS
L-AChBP_T2. NILEVNEITNEVDVVFVWQTTWSDRTLA--WNSSHSPDQVSVPISSLWVPDLAAYNAIS
A1_human QLINVDEVNQIVTTNVRLLKQWVDYNLKWNPDDYGGVKKIHIPSEKIWRPDLVLYNNADG
A7_human QIMDVDEKNQVLTNTNIWLQMSWTDHYLQWNVSEYPGVKTVRFPDQGIWKPDILLYNSADE
      : : : . . : * . . . : . * . : * * : * *

B-AChBP_T1. APELLSADRVVSKDGSVIYVPSQRVRFTCDLINVDTEPG-ATCRIKVGSWTHDNKQFAL
B-AChBP_T2. APELLSTDRVVVSKDGSVIYVPSQRVRFTCDLINVDTEPG-ATCRIKVGSWTFDNKQFAL
L-AChBP_T1. KPEVLTTPQLARVVSDGEVLYMPSIRQRFSCDVSGVDTESG-ATCRIKIGSWTHHSREISV
L-AChBP_T2. KPEVLTTPQLARVVSDGEVLYMPSIRQRFSCDVSGVDTESG-ATCRIKIGSWTHHSREISV
A1_human DFAIVKFTKVLLQYTGHTWTPPAIFKSYCEIIVTHFFDEQNCMSMKLGTWYDGSVVAI
A7_human RFDATFHTNVLVNSSGHCQYLPPIGIFKSSCYIDVRWFPPDVQHCKLKFGSWSYGG--WSL
      . : * : * . : * : . * : * : * : . :

B-AChBP_T1. ITGEEGVVNIAEYFDS-PKFDLLSATQSLNRKKYSCC-ENMYDDIEITFAFRKK-----
B-AChBP_T2. ITGEEGVVNIAEYFDS-PKYDLLSATQSLNRKKYRCC-ENMYEDIEITFAFRKK-----
L-AChBP_T1. DPTTE-NSDDSEYFSQYSRFEILDVTQKKNSVTYSCC-PEAYEDVEVSLNFRKKGRSEIL
L-AChBP_T2. DPTTE-NSDDSEYFSQYSRFEILDVTQKKNSVIYSCC-PEAYEDVEVSLNFRKKGRSEIL
A1_human NPESD-QPDLNFMES-GEWVIKESRGWKHSVTYSCCPDTPYLDITYHFVMQRLPLYFIV
A7_human DLQMQ-EADISGYIPN-GEWDLVGIPGKRSERFYECC-KEPYPDVTFVTMRRRTLYYGL
      : : : : . . : * * * * : . :

B-AChBP_T1. -----
B-AChBP_T2. -----
L-AChBP_T1. -----
L-AChBP_T2. -----
A1_human NVII PCLLFSFLTGLVFYLPDTSGEKMTLSISVLLSLTVFLLVIVELIPSTSSAVPLIGK
A7_human NLLI PCVLISALALLVFLLPADSGEKISLGITVLLSLTVFMLLVAEIMPATSDSVPLIAQ

B-AChBP_T1. -----
B-AChBP_T2. -----
L-AChBP_T1. -----
L-AChBP_T2. -----
A1_human YMLFTMVFVIASIIITVIVINTHHRSPSTHVMPNWRKVFI DTIPNIMFFSTMKRPSREK
A7_human YFASTMIIVGLSVVVTIVIVLQYHHHDPDGGKMPKWTRVILLN--WCAWFLRMKRPGEDK

B-AChBP_T1. -----
B-AChBP_T2. -----
L-AChBP_T1. -----
L-AChBP_T2. -----
A1_human Q-----DKKIFTEDIDISDISGKPGP-----PPMG-----
A7_human VRPACQHKQRRCSLASVEMSAVGPPPASNGNLLYIGFRGLDGVHCVPTPDSGVVCGRMAC

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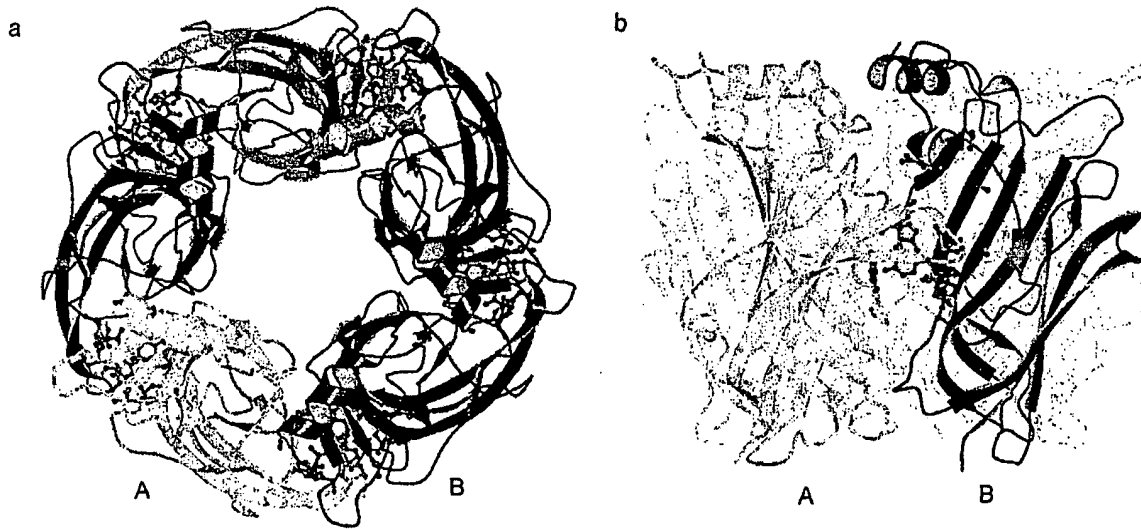
Figure 5

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| | |
|-------------|--|
| B-AChBP_T1. | ----- |
| B-AChBP_T2. | ----- |
| L-AChBP_T1. | ----- |
| L-AChBP_T2. | ----- |
| A1_human | -----FHS--PLIKHPEVKSAIEGIKYIAETMKSDQESNNAAEWKYVAMVMDHILL |
| A7_human | SPTHDEHLLHGGQPPEGDPDLAKILEEVRYIANRFRQCDESEAVCSEWKFAACVVDRLCL |
| | |
| B-AChBP_T1. | ----- |
| B-AChBP_T2. | ----- |
| L-AChBP_T1. | ----- |
| L-AChBP_T2. | ----- |
| A1_human | GVFMLVCIIGTLAVFAGR--LIELNQOG--- |
| A7_human | MAFSVFTIICTIGILMSAPNFVEAVSKDFAZ |

Figure 5 (continued)

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**Figure 6**

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Figure 8

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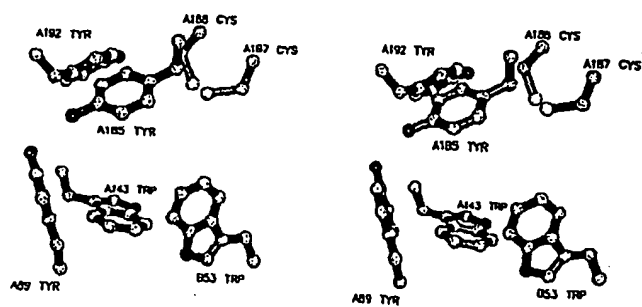


Figure 9

Figure 10

Figure 11

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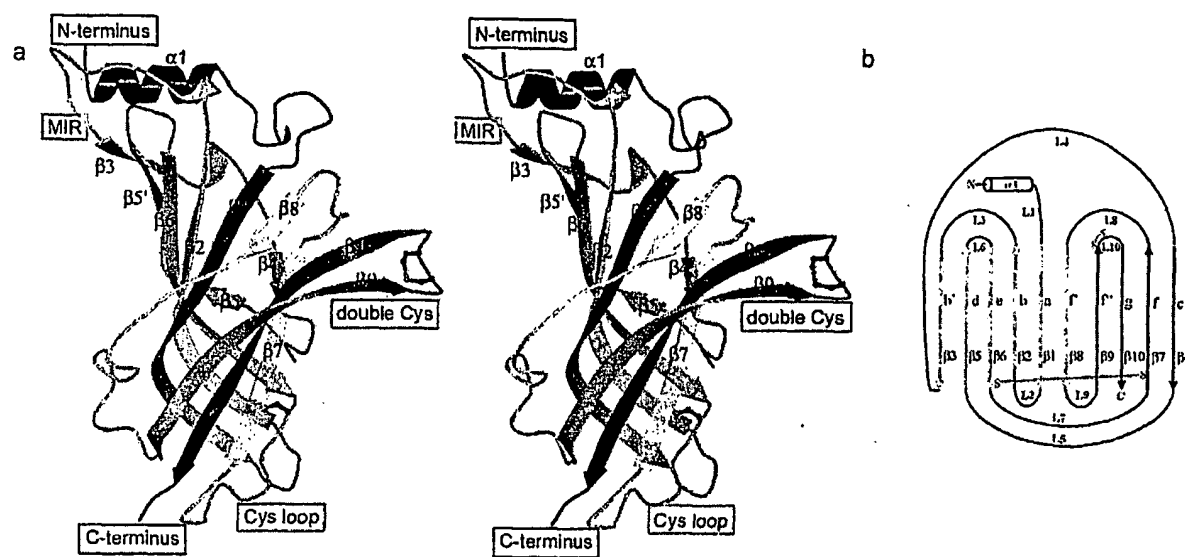


Figure 12

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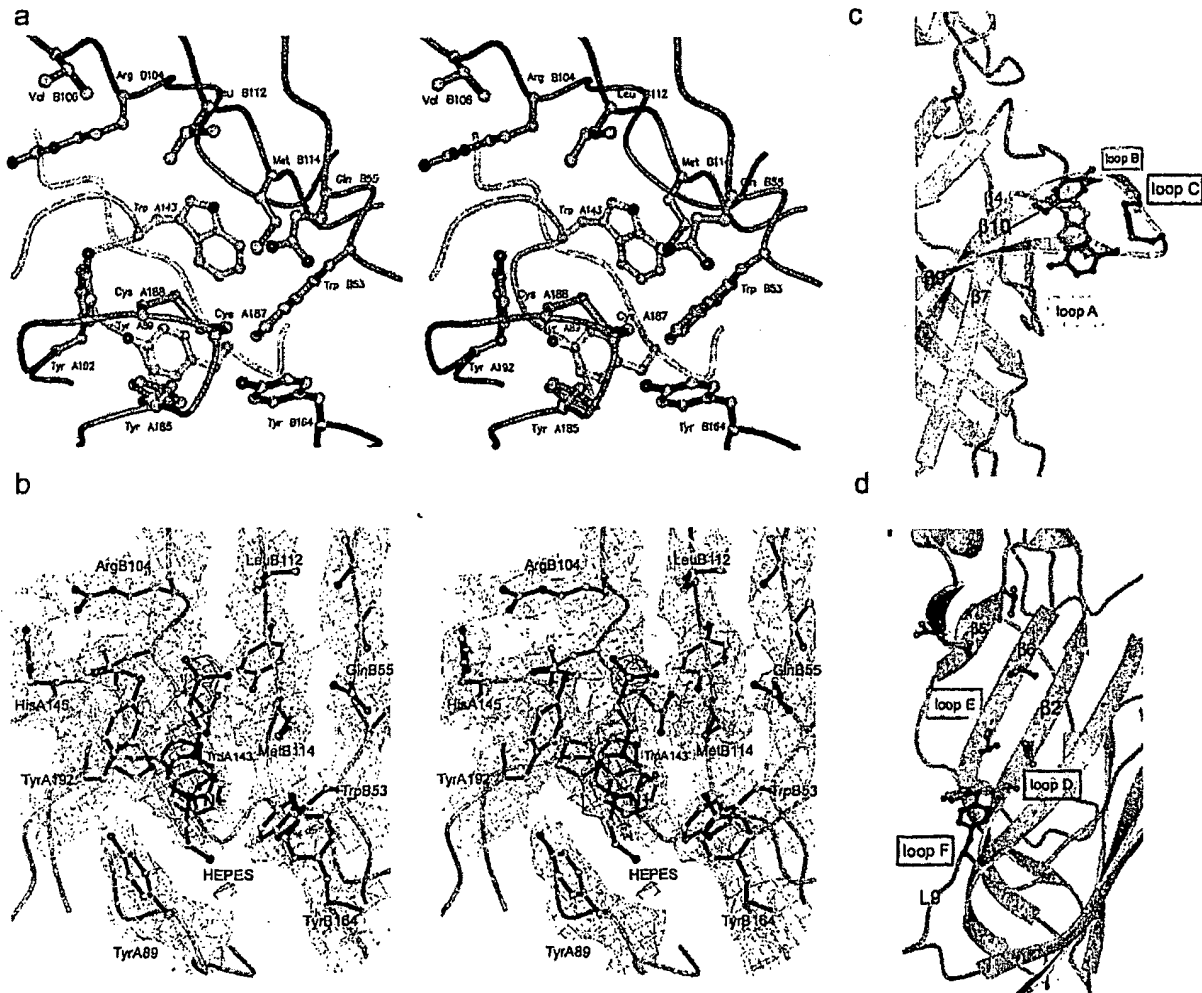


Figure 13

(18/19)

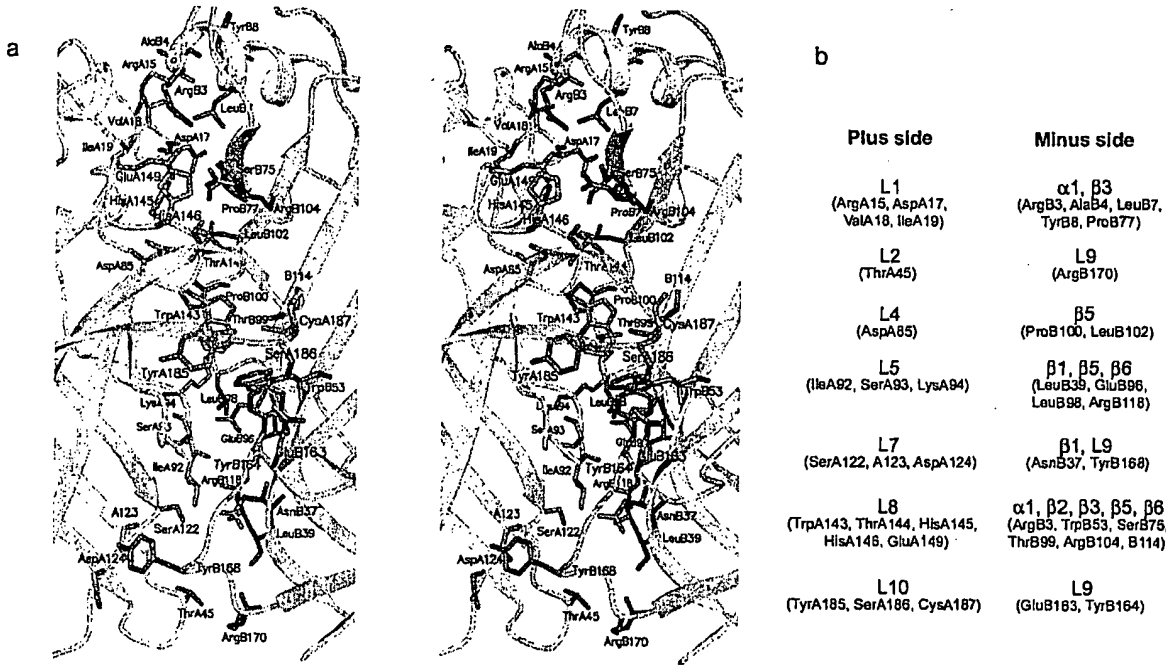
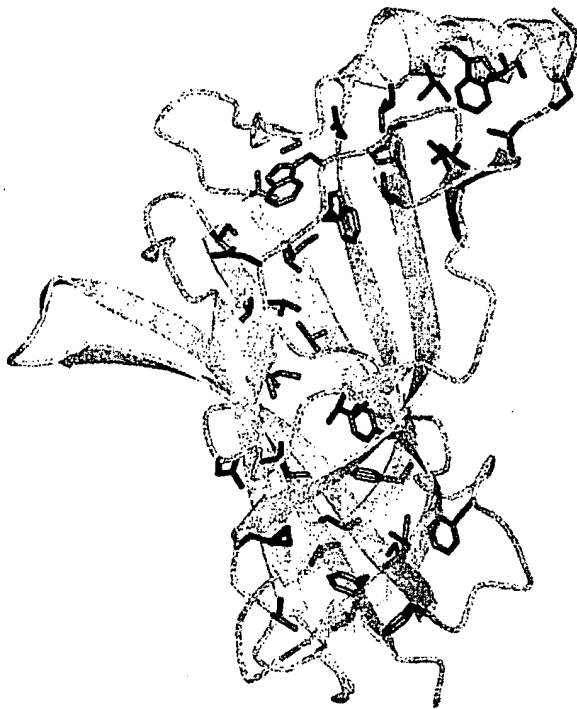


Figure 14

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**Figure 15**

(1/20)

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(2/20)

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| 80 85 90 | |
| aaa cct gaa gtc ctt aca ccg caa ctg gcc agg gtc gta tcc gat ggt | 384 |
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(3/20)

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Ile Ser Ser Leu Trp Val Pro Asp Leu Ala Ala Tyr Asn Ala Ile Ser
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(4/20)

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(6/20)

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(7/20)

| | | |
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| 110 | 115 | 120 |
| Ser Gly Val Asp Thr Glu Ser Gly Ala Thr Cys Arg Ile Lys Ile Gly | | |
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| Ser Trp Thr His His Ser Gly Glu Ile Ser Val Asp Pro Thr Thr Glu | | |
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| Asn Ser Asp Asp Ser Glu Tyr Phe Ser Gln Tyr Ser Arg Phe Glu Ile | | |
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| Leu Asp Val Thr Gln Lys Lys Asn Ser Val Ile Tyr Ser Cys Cys Pro | | |
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 15 20 25

tcg ctg aat ttt aag ctg atg aat atc gta gag gcg gac aca gaa aaa 192
 Ser Leu Asn Phe Lys Leu Met Asn Ile Val Glu Ala Asp Thr Glu Lys
 30 35 40

gat caa gtg gag gtc gtg ctg tgg aca cag gct agc tgg aaa gtg ccg 240
 Asp Gln Val Glu Val Val Leu Trp Thr Gln Ala Ser Trp Lys Val Pro
 45 50 55

tat tac agc tca ctg ctg tcc tct agc agt tta gac cag gtg agc tta 288
 Tyr Tyr Ser Ser Leu Leu Ser Ser Ser Ser Leu Asp Gln Val Ser Leu
 60 65 70 75

cca gtc agc aaa atg tgg acc cca gac ctt tct ttc tac aac gcc atc 336
 Pro Val Ser Lys Met Trp Thr Pro Asp Leu Ser Phe Tyr Asn Ala Ile
 80 85 90

gct gca ccc gag ttg ctc tcc gca gac cgc gtg gtg gtc tct aag gac 384
 Ala Ala Pro Glu Leu Leu Ser Ala Asp Arg Val Val Val Ser Lys Asp
 95 100 105

(9/20)

ggg agc gtc att tac gtc ccc agc cag agg gtc cgt ttc acc tgc gac 432
 Gly Ser Val Ile Tyr Val Pro Ser Gln Arg Val Arg Phe Thr Cys Asp
 110 115 120

ctt att aat gtc gac acg gag ccg gga gcc acc tgt cgc atc aaa gtc 480
 Leu Ile Asn Val Asp Thr Glu Pro Gly Ala Thr Cys Arg Ile Lys Val
 125 130 135

gga tcc tgg acc cac gac aac aaa cag ttc gcc ctg atc acc ggg gag 528
 Gly Ser Trp Thr His Asp Asn Lys Gln Phe Ala Leu Ile Thr Gly Glu
 140 145 150 155

gag ggg gtg gtg aat att gca gag tac ttc gac agc cca aag ttt gac 576
 Glu Gly Val Val Asn Ile Ala Glu Tyr Phe Asp Ser Pro Lys Phe Asp
 160 165 170

ctt ttg agt gcc aca cag agt ctg aat cgc aag aag tac agc tgt tgc 624
 Leu Leu Ser Ala Thr Gln Ser Leu Asn Arg Lys Lys Tyr Ser Cys Cys
 175 180 185

gag aat atg tat gat gac att gaa att acc ttt gca ttc aga aag aag 672
 Glu Asn Met Tyr Asp Asp Ile Glu Ile Thr Phe Ala Phe Arg Lys Lys
 190 195 200

taa 675

<210> 6

<211> 224

<212> PRT

<213> *Bulinus truncatus*

<400> 6

Met Ala Glu Leu Arg Arg Ile Ile Leu Leu Leu Cys Thr Ile Ala Phe
 -20 -15 -10

His Val Ser His Gly Gln Ile Arg Trp Thr Leu Leu Asn Gln Ile Thr
 -5 -1 1 5 10

Gly Glu Ser Asp Val Ile Pro Leu Ser Asn Asn Thr Pro Leu Asn Val

(10/20)

| | | | | | |
|-----|-----|-----|-----|-----|-----|
| | 15 | | 20 | | 25 |
| Ser | Leu | Asn | Phe | Lys | Leu |
| | 30 | | 35 | | 40 |
| Met | Asn | Ile | Val | Glu | Ala |
| | | | | | |
| Asp | Thr | Glu | Lys | | |
| | | | | | |
| Asp | Gln | Val | Glu | Val | Val |
| | 45 | | 50 | | 55 |
| Leu | Trp | Thr | Gln | Ala | Ser |
| | | | | | |
| Trp | Lys | Val | Pro | | |
| | | | | | |
| Tyr | Tyr | Ser | Ser | Leu | Leu |
| | 60 | | 65 | | 70 |
| Ser | Ser | Ser | Ser | Leu | Asp |
| | | | | | |
| Gln | Val | Ser | Leu | | |
| | | | | | |
| Pro | Val | Ser | Lys | Met | Trp |
| | | | 80 | | |
| Thr | Pro | Asp | Leu | Ser | Phe |
| | | | | | |
| Tyr | Asn | Ala | Ile | | |
| | | | | | |
| Ala | Ala | Pro | Glu | Leu | Leu |
| | 95 | | 100 | | 105 |
| Ser | Ala | Asp | Arg | Val | Val |
| | | | | | |
| Val | Val | Ser | Lys | Asp | |
| | | | | | |
| Gly | Ser | Val | Ile | Tyr | Val |
| | 110 | | 115 | | 120 |
| Pro | Ser | Gln | Arg | Val | Arg |
| | | | | | |
| Phe | Thr | Cys | Asp | | |
| | | | | | |
| Leu | Ile | Asn | Val | Asp | Thr |
| | 125 | | 130 | | 135 |
| Glu | Pro | Gly | Ala | Thr | Cys |
| | | | | | |
| Arg | Ile | Lys | Val | | |
| | | | | | |
| Gly | Ser | Trp | Thr | His | Asp |
| | 140 | | 145 | | 150 |
| Asn | Lys | Gln | Phe | Ala | Leu |
| | | | | | |
| Ile | Thr | Gly | Glu | | |
| | | | | | |
| Glu | Gly | Val | Val | Asn | Ile |
| | | | | | |
| Ala | Glu | Tyr | Phe | Asp | Ser |
| | 160 | | 165 | | 170 |
| Pro | Lys | Phe | Asp | | |
| | | | | | |
| Leu | Leu | Ser | Ala | Thr | Gln |
| | 175 | | 180 | | 185 |
| Ser | Leu | Asn | Arg | Lys | Lys |
| | | | | | |
| Tyr | Ser | Cys | Cys | | |
| | | | | | |
| Glu | Asn | Met | Tyr | Asp | Asp |
| | 190 | | 195 | | 200 |
| Ile | Glu | Ile | Thr | Phe | Ala |
| | | | | | |
| Phe | Arg | Lys | Lys | | |
| | | | | | |

<210> 7

<211> 675

<212> DNA

(11/20)

<213> *Bulinus truncatus*

<220>

<221> CDS

<222> (1)..(672)

<220>

<221> mat_peptide

<222> (64)..(672)

<400> 7

atg gct gaa cta cga ggg atc att ctt ctg cta tgt act att gcc ttt 48

Met Ala Glu Leu Arg Gly Ile Ile Leu Leu Leu Cys Thr Ile Ala Phe

-20

-15

-10

cat gtt tcc cat gga caa ata aga tgg acg ctg ctg aat cag atc acc 96

His Val Ser His Gly Gln Ile Arg Trp Thr Leu Leu Asn Gln Ile Thr

-5

-1 1

5

10

ggc gaa tct gac gtc att ccg ctg tct aac aac acg cca ctg aat gtg 144

Gly Glu Ser Asp Val Ile Pro Leu Ser Asn Asn Thr Pro Leu Asn Val

15

20

25

tcg ctg aat ttt aag ctg atg aat atc tta gag gcg gac aca gag aaa 192

Ser Leu Asn Phe Lys Leu Met Asn Ile Leu Glu Ala Asp Thr Glu Lys

30

35

40

gat caa gtg gag gtc gtg ctg tgg aca cag gct agc tgg aaa gtg ccg 240

Asp Gln Val Glu Val Val Leu Trp Thr Gln Ala Ser Trp Lys Val Pro

45

50

55

tat tac agc tca ctg ctg tcc tct agc agt tta gac cag gtg agc tta 288

Tyr Tyr Ser Ser Leu Leu Ser Ser Ser Ser Leu Asp Gln Val Ser Leu

60

65

70

75

cca gcc agc aaa atg tgg acc cca gac ctt tct ttc tat aac gcc atc 336

Pro Ala Ser Lys Met Trp Thr Pro Asp Leu Ser Phe Tyr Asn Ala Ile

80

85

90

gct gca ccc gag ttg ctc tcc aca gac cgc gtg gtg gtc tct aag gac 384

(12/20)

Ala Ala Pro Glu Leu Leu Ser Thr Asp Arg Val Val Val Ser Lys Asp
 95 100 105

ggg agc gtc att tac gtg ccc agc cag agg gtc cgt ttc acc tgc gac 432
 Gly Ser Val Ile Tyr Val Pro Ser Gln Arg Val Arg Phe Thr Cys Asp
 110 115 120

ctt att aat gtg gac acg gag ccg gga gcc acc tgt cgc atc aaa gtc 480
 Leu Ile Asn Val Asp Thr Glu Pro Gly Ala Thr Cys Arg Ile Lys Val
 125 130 135

gga tcc tgg acc ttc gac aac aaa cag ctc gcc ctg atc acc ggg gag 528
 Gly Ser Trp Thr Phe Asp Asn Lys Gln Leu Ala Leu Ile Thr Gly Glu
 140 145 150 155

gag ggg gtg gtg aat att gca gag tac ttc gac agc cca aag tac gac 576
 Glu Gly Val Val Asn Ile Ala Glu Tyr Phe Asp Ser Pro Lys Tyr Asp
 160 165 170

ctt ttg agt gcc aca cag agt ctg aat cgc aag aag tac aga tgt tgc 624
 Leu Leu Ser Ala Thr Gln Ser Leu Asn Arg Lys Lys Tyr Arg Cys Cys
 175 180 185

gag aat atg tat gaa gac att gaa att acc ttt gca ttc aga aag aag 672
 Glu Asn Met Tyr Glu Asp Ile Glu Ile Thr Phe Ala Phe Arg Lys Lys
 190 195 200

taa 675

<210> 8

<211> 224

<212> PRT

<213> Bulinus truncatus

<400> 8

Met Ala Glu Leu Arg Gly Ile Ile Leu Leu Leu Cys Thr Ile Ala Phe
 -20 -15 -10

His Val Ser His Gly Gln Ile Arg Trp Thr Leu Leu Asn Gln Ile Thr

(13/20)

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| -5 | -1 | 1 | | 5 | | 10 | | | | | | | | | |
| Gly | Glu | Ser | Asp | Val | Ile | Pro | Leu | Ser | Asn | Asn | Thr | Pro | Leu | Asn | Val |
| | | | 15 | | | | | | 20 | | | | 25 | | |
| Ser | Leu | Asn | Phe | Lys | Leu | Met | Asn | Ile | Leu | Glu | Ala | Asp | Thr | Glu | Lys |
| | | 30 | | | | | | 35 | | | | | 40 | | |
| Asp | Gln | Val | Glu | Val | Val | Leu | Trp | Thr | Gln | Ala | Ser | Trp | Lys | Val | Pro |
| | 45 | | | | | | | 50 | | | | 55 | | | |
| Tyr | Tyr | Ser | Ser | Leu | Leu | Ser | Ser | Ser | Ser | Ser | Leu | Asp | Gln | Val | Ser |
| 60 | | | | | 65 | | | | | | 70 | | | | 75 |
| Pro | Ala | Ser | Lys | Met | Trp | Thr | Pro | Asp | Leu | Ser | Phe | Tyr | Asn | Ala | Ile |
| | | | | 80 | | | | | 85 | | | | | 90 | |
| Ala | Ala | Pro | Glu | Leu | Leu | Ser | Thr | Asp | Arg | Val | Val | Val | Ser | Lys | Asp |
| | | | 95 | | | | | | 100 | | | | | 105 | |
| Gly | Ser | Val | Ile | Tyr | Val | Pro | Ser | Gln | Arg | Val | Arg | Phe | Thr | Cys | Asp |
| | | 110 | | | | | | | 115 | | | | 120 | | |
| Leu | Ile | Asn | Val | Asp | Thr | Glu | Pro | Gly | Ala | Thr | Cys | Arg | Ile | Lys | Val |
| | 125 | | | | | | | 130 | | | | 135 | | | |
| Gly | Ser | Trp | Thr | Phe | Asp | Asn | Lys | Gln | Leu | Ala | Leu | Ile | Thr | Gly | Glu |
| 140 | | | | | 145 | | | | | 150 | | | | 155 | |
| Glu | Gly | Val | Val | Asn | Ile | Ala | Glu | Tyr | Phe | Asp | Ser | Pro | Lys | Tyr | Asp |
| | | | 160 | | | | | | 165 | | | | | 170 | |
| Leu | Leu | Ser | Ala | Thr | Gln | Ser | Leu | Asn | Arg | Lys | Lys | Tyr | Arg | Cys | Cys |
| | | | 175 | | | | | | 180 | | | | | 185 | |
| Glu | Asn | Met | Tyr | Glu | Asp | Ile | Glu | Ile | Thr | Phe | Ala | Phe | Arg | Lys | Lys |
| | | 190 | | | | | | | 195 | | | | | 200 | |

(14/20)

<210> 9

<211> 502

<212> PRT

<213> Homo sapiens

<220>

<221> DOMAIN

<222> (1)..(235)

<400> 9

Met Arg Cys Ser Pro Gly Gly Val Trp Leu Ala Leu Ala Ala Ser Leu
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Leu His Val Ser Leu Gln Gly Glu Phe Gln Arg Lys Leu Tyr Lys Glu
 20 25 30

Leu Val Lys Asn Tyr Asn Pro Leu Glu Arg Pro Val Ala Asn Asp Ser
 35 40 45

Gln Pro Leu Thr Val Tyr Phe Ser Leu Ser Leu Leu Gln Ile Met Asp
 50 55 60

Val Asp Glu Lys Asn Gln Val Leu Thr Thr Asn Ile Trp Leu Gln Met
 65 70 75 80

Ser Trp Thr Asp His Tyr Leu Gln Trp Asn Val Ser Glu Tyr Pro Gly
 85 90 95

Val Lys Thr Val Arg Phe Pro Asp Gly Gln Ile Trp Lys Pro Asp Ile
 100 105 110

Leu Leu Tyr Asn Ser Ala Asp Glu Arg Phe Asp Ala Thr Phe His Thr
 115 120 125

Asn Val Leu Val Asn Ser Ser Gly His Cys Gln Tyr Leu Pro Pro Gly
 130 135 140

Ile Phe Lys Ser Ser Cys Tyr Ile Asp Val Arg Trp Phe Pro Phe Asp
 145 150 155 160

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Val Gln His Cys Lys Leu Lys Phe Gly Ser Trp Ser Tyr Gly Gly Trp
 165 170 175

Ser Leu Asp Leu Gln Met Gln Glu Ala Asp Ile Ser Gly Tyr Ile Pro
 180 185 190

Asn Gly Glu Trp Asp Leu Val Gly Ile Pro Gly Lys Arg Ser Glu Arg
 195 200 205

Phe Tyr Glu Cys Cys Lys Glu Pro Tyr Pro Asp Val Thr Phe Thr Val
 210 215 220

Thr Met Arg Arg Arg Thr Leu Tyr Tyr Gly Leu Asn Leu Leu Ile Pro
 225 230 235 240

Cys Val Leu Ile Ser Ala Leu Ala Leu Leu Val Phe Leu Leu Pro Ala
 245 250 255

Asp Ser Gly Glu Lys Ile Ser Leu Gly Ile Thr Val Leu Leu Ser Leu
 260 265 270

Thr Val Phe Met Leu Leu Val Ala Glu Ile Met Pro Ala Thr Ser Asp
 275 280 285

Ser Val Pro Leu Ile Ala Gln Tyr Phe Ala Ser Thr Met Ile Ile Val
 290 295 300

Gly Leu Ser Val Val Val Thr Val Ile Val Leu Gln Tyr His His His
 305 310 315 320

Asp Pro Asp Gly Gly Lys Met Pro Lys Trp Thr Arg Val Ile Leu Leu
 325 330 335

Asn Trp Cys Ala Trp Phe Leu Arg Met Lys Arg Pro Gly Glu Asp Lys
 340 345 350

Val Arg Pro Ala Cys Gln His Lys Gln Arg Arg Cys Ser Leu Ala Ser
 355 360 365

Val Glu Met Ser Ala Val Ala Pro Pro Pro Ala Ser Asn Gly Asn Leu

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| | | |
|---|-----|---------|
| 370 | 375 | 380 |
| Leu Tyr Ile Gly Phe Arg Gly Leu Asp Gly Val His Cys Val Pro Thr | | |
| 385 | 390 | 395 400 |
| Pro Asp Ser Gly Val Val Cys Gly Arg Met Ala Cys Ser Pro Thr His | | |
| 405 | 410 | 415 |
| Asp Glu His Leu Leu His Gly Gly Gln Pro Pro Glu Gly Asp Pro Asp | | |
| 420 | 425 | 430 |
| Leu Ala Lys Ile Leu Glu Glu Val Arg Tyr Ile Ala Asn Arg Phe Arg | | |
| 435 | 440 | 445 |
| Cys Gln Asp Glu Ser Glu Ala Val Cys Ser Glu Trp Lys Phe Ala Ala | | |
| 450 | 455 | 460 |
| Cys Val Val Asp Arg Leu Cys Leu Met Ala Phe Ser Val Phe Thr Ile | | |
| 465 | 470 | 475 480 |
| Ile Cys Thr Ile Gly Ile Leu Met Ser Ala Pro Asn Phe Val Glu Ala | | |
| 485 | 490 | 495 |
| Val Ser Lys Asp Phe Ala | | |
| 500 | | |

<210> 10

<211> 10

<212> PRT

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: N-terminus of
mature LACHBP1

<400> 10

| |
|---|
| Leu Asp Arg Ala Asp Ile Leu Tyr Asn Ile |
| 1 5 10 |

(17/20)

<210> 11

<211> 32

<212> DNA

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence:

Oligonucleotides encoding N-terminal peptide of
LACHBP1

<220>

<221> modified_base

<222> (13)

<223> i

<400> 11

cggatccgay mgagcngaya thytntayaa ya

32

<210> 12

<211> 31

<212> DNA

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Primer1 useful
for cloning cDNA encoding LACHBP (optionally with
Primer2)

<220>

<221> modified_base

<222> (14)

<223> i

<220>

<221> modified_base

<222> (20)

<223> i

(18/20)

<400> 12

gcgaattcga yacagarwsa ggngcnacnt g

31

<210> 13

<211> 33

<212> DNA

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Primer2
useful for cloning cDNA encoding LACHBP
(optionally with Primer1)

<220>

<221> modified_base

<222> (20)

<223> 1

<400> 13

gcgaagcttc rtcytcrtaa gcytcngcrc arc

33

<210> 14

<211> 9

<212> PRT

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: His-tag

<400> 14

Ser Arg Gly His His His His His His

1

5

<210> 15

<211> 14

<212> PRT

<213> Artificial Sequence

(19/20)

<220>

<223> Description of Artificial Sequence: His-tag

<400> 15

Glu Phe Lys Asp Asp Asp Asp Lys His His His His His His
1 5 10

<210> 16

<211> 4

<212> PRT

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Additonal
amino acids at the N-terminus of mature LChBP due
to alpha-mating factor cleavage site

<400> 16

Glu Ala Glu Ala
1

<210> 17

<211> 47

<212> DNA

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Primer useful
for generating LChBP/alpha7 nChR chimera

<400> 17

gcgctcgaga aaagagaggc tgaagctttg gaccgggcag acatctt

47

<210> 18

<211> 30

<212> DNA

(20/20)

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Primer useful
for generating LChBP/alpha7 nACHR chimera

<400> 18

cgcggaattca agaatttcgg agcgtccctt

30

<210> 19

<211> 42

<212> DNA

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Primer useful
for generating LChBP/alpha7 nACHR chimera

<400> 19

gtggaaacca gacattctcc tctacaacgc catctcgaaa cc

42

<210> 20

<211> 39

<212> DNA

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Primer useful
for generating LChBP/alpha7 nACHR chimera

<400> 20

gaggagaatg tctggtttcc acaaagagct tattggcac

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